**ADDITIONS AND CORRECTIONS TO SUPPLEMENT A2.pdf**

**SOME PRELIMINARY NOTES to the ADDITIONS**

|  |
| --- |
| **1 Pa = 0.0075 mm Hg, or 1 mm Hg = 133.3 Pa == 1 torr; 100 000 Pa == 1 bar**  **1 Pa = 1 N/m2= 1 J/m3**  **1 atm = 760 mm Hg = 101 325 Pa** |

|  |
| --- |
| **ΔH is always given here in kJ/mol** (but for the energies of torsional angles, taken from [A1] , which are in kcal/mol)  **P is always given here in Pa = N/m2 = J/m3**  **T is in deg. C (unless otherwise indicated)** |

|  |
| --- |
| Henry's Law Constants:  **1) Leonid’s designations:**  kH,cp, expressed usually in[(mol/L in liquid)/(atm in gas)]; kH,cc ≡ [in liquid]/[in gas]= kH,cp×RT [dimensionless]  If kH,cp= κ in [(mol/L)/atm], then kH,cp= κ⋅0.00987 in [mol/J]  (because [(mol/L)/atm] = [(mol/L)/(101 325 Pa)] = [(mol/L)/(101 325 J/m3)] = [(mol/L)/(101.325 J/L)] = [(mol/L)/(101.325 J/L)] = 0.00987 in [mol/J]).  T = 25oC = 298.15K, where RT = 2478.66 [J/mol]:  kH,cc = kH,cp×RT = κ⋅0.00987 [mol/J] × 2478.66 [J/mol] = κ⋅24.62; kH,cc = exp[-(G0in liquid – G0in gas)/RT] = exp[-G0in liquid/RT]  ln(kH,cc) = ln(kH,cc) + 3.20  **2) Conversion to universal SI units:**  kH,cc = limC→0 {Caq/Cgas} [dimensionless]= limC→0 {Caq/(Pgas/RT)} = RT/limC→0 {Pgas/Caq} = RT/kH,pc  kH,pc = limC→0 {Pgas/Caq}; usually measured either in [(atm in gas)/(mol/m3 in liquid)] (then, designated as kH,pc,atm×m3)  or in [(Pa in gas)/(mol/L in liquid)] (then, designated as kH,pc,Pa×L)  In SI units: [(Pa in gas)/(mol/m3 in liquid)] = [Pa×m3/mol] ≡ [J/mol]. Thus, kH,pc,SI measured in [J/mol] units.  Then kH,pc,SI = 101 325 [atm/Pa]×kH,pc,atm×m3 = 101 325×kH,pc,atm×m3 = 0.001 [L/m3]×kH,pc,Pa×L = 0.001×kH,pc,Pa×L in [J/mol]  kH,cc = RT/kH,pc,SI. At T=25oC => 298.15K, RT = 2478.66 [J/mol], or kH,cc(25C) = RT25C/kH,pc,SI(25C) = 2478.66/kH,pc,SI(25C) |

**1 Methylamine**

 Ko=3

lever arm of the **H3C—NH2** bond: 1.0sin120o=0.87A

K1=2, n1=6

??-N?-C?-?? 0 [A1]

Melting Temperature(C) **-93.4** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **36.695** ± 0.210 **SOLID**

Vapor pressure 2.65X10+3 mm Hg = **353245 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **23.37** [A6] ***LIQUID***

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 1 | -93.4 | A3 | 36.695 | - | - | 0.08 | A2 | 353245 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**2 Ethanol**

 Ko=1

lever arm of the **H3C—C-O** bond: 1.09sin109.5o=1.03A

K1=3, n1=3

??-C?-C?-?? 1.4

lever arm of the **C-C—O-H** bond: 1.0sin109.5o=0.94A

K2=1, n2=3

??-C?-O?-?? 0.6 [A1]

Melting Temperature(C) **-114.1** [A3]

**[A2}:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **53.807**±3.597 **SOLID**

Vapor pressure 59.3 mm Hg = **7905 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **42.32** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 2 | -114.1 | A3 | 53.807 | - | - | 1.4 | A2 | 7905 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**3 Dimethyl sulfide**

 Ko=2

lever arm of the **H3C—S-C** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-S?-C?-?? 1.0 [A1]

Melting Temperature(C) **-98.24** [A4][

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **39.567** ± 1.682 **SOLID**

Vapor pressure 502 mm Hg = **66917 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **28.15** obtained from interpolation of pressure-temperature dependence (-96 - +37C, [A4]) *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 3 | -98.24 | A4 | 39.567 | - | - | 0.7 | A2 | 66917 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**4 Dimethyl disulfide**

 Ko=2

lever arm of the **H3C—S-S** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

S?-S?-C?-?? 0

lever arm of the **C-S—S-C** bond: (1.09+.6845+1.389+.6845+1.389)sin120o=5.26A

K2=1, n2=2

??-S?-S?-?? 6 [A1]

Melting Temperature(C) **-84.67** [A4][

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **54.024** ± 4.9 **SOLID**

Vapor pressure 28.7 mm Hg = **3826 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **38.515** obtained from interpolation of pressure-temperature dependence (-71 - +109.3C [A4][) *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 4 | -84.67 | A4 | 54.024 | - | - | 2 | A2 | 3826 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**5 Cyclopropane**

**Rigid** [A1]  **** Ko=6

Melting Temperature(C) **-124** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **26.26** ± 0. 11 **SOLID**

Vapor pressure 5.41X10+3 mm Hg = **721153 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **16.93** [A6]*LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 5 | -124 | A3 | 26.26 | - | - | 0.04 | A2 | 721153 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**6 Acetone**

 Ko=2

lever arm of the **H3C—CO-C** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1 [A1]

Melting Temperature(C) **-94.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **39.85** ± 0. 48 **SOLID**

Vapor pressure 231 mm Hg = **30792 Pa** at 25 deg C[A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **32.08** obtained from interpolation of pressure-temperature dependence (-95 – +55.7C [A7]) *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 6 | -94.8 | A3 | 39.85 | - | - | 0.19 | A2 | 30792 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**7 Trioxane (1,3,5 Trioxane, s-Trioxane)**

**Rigid** [A1] Ko=12 = 6x2 not flat

Melting Temperature(C)  **+60.29** [A4]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **56.10** ± 0. 46 [A8, A9] **SOLID**

ΔHsubl[25C] = **55.6, 56.5, 56.2** ± 0:2 [A8, A9]

**ΔHsubl[25C]=56.568** [A10] **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **55. ± 6.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 6 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C110883&Units=SI&Type=HSUBLIME) |

Vapor Pressure (mm Hg @ 25oC) 13 = **1733 Pa** [A11]; nothing in [A5] **SOLID**

Vapor Pressure: 17.3 mbar = **1730** Pa @ 25 oC [A12] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 7 | 60.29 | A4 | 56.0 | 55.6 | 56.568 | 1.1 | A8,A9,A10,A13 | 1731.5 | 1730 | 1733 | 0.001 | A11,A12 |

**DATA on SOLUBILITY and**

**r HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**8 Trimethylamine**

 Ko=12 - not flat

lever arm of the **H3C—N-C** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (THREE SUCH BONDS)

??-N?-C?-?? 0 [A1]

Melting Temperature(C) **-117.1** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **34.628** ± 1.857 ] **SOLID**

Vapor pressure 1610 mm Hg = **214613 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **21.66** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 8 | -117.1 | A3 | 34.628 | - | - | 0.74 | A2 | 214613 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**9 Succinic Anhydride**

**Rigid** [A1]  **** Ko=2 - flat

Melting Temperature(C) **119** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 81.1 ± 1.6 **SOLID**

**80.7 ± 1.6** [A8, A9]  **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13] ΔsubH° | **80.7 ± 1.6** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Meng-Yan and Pilcher, 1990](http://webbook.nist.gov/cgi/cbook.cgi?Name=Succinic+Anhydride&Units=SI&cTP=on#ref-5) | AC |
| [A13] ΔsubH° | **80.7 ± 1.6** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Yan and Pilcher, 1990](http://webbook.nist.gov/cgi/cbook.cgi?Name=Succinic+Anhydride&Units=SI&cTP=on#ref-6) | ALS |
| [A13] ΔsubH° | **80.7** | kJ/mol | N/A | [Yan and Pilcher, 1990](http://webbook.nist.gov/cgi/cbook.cgi?Name=Succinic+Anhydride&Units=SI&cTP=on#ref-6) | DRB |

**[A2]:** vapor pressure at 25 deg C **4.022 Pa** extrapolation of P-T dependence [16] (121-260, liquid >> 25oC) **SOLID**

vapor pressure at 25 deg C 1.5X10-3 mm Hg = **0.200 Pa** [A5], [A14] **SOLID**

Vapour pressure, Pa at *T*0\*=92°C: 1300 [A5]

 = -5.97;

= **3.31 Pa** at 25oC  **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 9 | 119 | A3 | 80.7 | 80.7 | 80.7 | 0.64 | A8,A9,A13 | 1.39 | 0.200 | 4.022 | 1.37 | A2,A5,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**10 Pyrrole (1H-Pyrrole)**

**Rigid** [A1]  **** Ko=2 - flat

Melting Temperature(C) **-23.4** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **55.38** ± 1.18 **SOLID**

vapor pressure at 25 deg C: 8.35 mm Hg = **1113 Pa** [A14] not found in [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **45.09** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 10 | -23.4 | A3 | 55.38 | - | - | 0.45 | A2 | 1113 | - | - | - | A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**11 Dimethyl Oxalate**

**** Ko=2

lever arm of the **H3C—O-C** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-O?-?? 0.6

lever arm of the **C-O—CO-C** bond: 1.437sin109.5o=1.35A

K1=1, n1=2 (TWO SUCH BONDS)

??-A?-O2-?? 1.8

lever arm of the **O-CO—CO-C** bond: 1.437sin120o=1.35A

K2=1, n2=2

**??-A?-A?-?? 10** [A1]

Melting Temperature(C) **54.35** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **74.95** ± 1.6 **[A8, A9]** **SOLID**

[A8, A9]: 74.6±0.7; 75.3±1.6 at 298

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **75.2 ± 0.5** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Chickos, Sabbah, et al., 1996](http://webbook.nist.gov/cgi/cbook.cgi?Name=Dimethyl+Oxalate+&Units=SI&cTP=on#ref-11) | ALS |
| ΔsubH° | **74.6 ± 0.7** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Chickos, Sabbah, et al., 1996](http://webbook.nist.gov/cgi/cbook.cgi?Name=Dimethyl+Oxalate+&Units=SI&cTP=on#ref-11) | AC |
| ΔsubH° | **75.3 ± 1.6** | kJ/mol | N/A | [Chickos, Sabbah, et al., 1996](http://webbook.nist.gov/cgi/cbook.cgi?Name=Dimethyl+Oxalate+&Units=SI&cTP=on#ref-11) | AC |
| ~~Δ~~~~sub~~~~H°~~ | ~~47.0~~ | ~~kJ/mol~~ | ~~N/A~~ | [~~Anthoney, Carson, et al., 1976, 2~~](http://webbook.nist.gov/cgi/cbook.cgi?Name=Dimethyl+Oxalate+&Units=SI&cTP=on#ref-12) | ~~DRB~~ “was in error”: Comment from  Chickos et al. Struct. Chem., 7, 391 (1996) |

ΔsubH = Δcr,g*H*m(298.15 K) = (**75.8** ± 0.53) kJ/mol; [A15] **SOLID**

T=298.2 P= **79.59** Pa [A15] **SOLID**

**P(**298.15 K**) = 192 Pa** [A13]; not found in [A5] **SOLID**

**[A2]:** **P(**25oC**) = 210 Pa** from P-T dependence from [A7] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 11 | 54.35 | A3 | 75.2 | 74.6 | 75.8 | 0.36 | A8,A9,A13,A15 | 147 | 79.59 | 210 | 0.44 | A2,A7A13,A15 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**12 Tetrahydrofuran**

**Rigid** [A1]  **** Ko= 4 = 2x2 not flat

Melting Temperature(C) **-108.3** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **46.807** ± 4.724 **SOLID**

=21037 Pa at 25oC *LIQUID* from P-T dependence from [A7] ***LIQUID***

**P(**298.15 K**) = 21623 Pa** [A13] ***LIQUID***

**P(**298.15 K**) =** 162 mm Hg at 25 deg C = **21594 Pa** [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **31.99** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 12 | -108.3 | A3 | 48.807 | - | - | 1.9 | A2 | 21608 | 21594 | 21623 | 0.0001 | A5,A7,A13 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**13 1,4-Dioxane**

**Rigid** [A1]  ** ** Ko=8 = 4x2 not flat; chair

Melting Temperature(C) 11.85 [A4]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **49.459** ± 0. 459 **SOLID**

ΔHmelt[25C](kJ/mol) 12.84 [A4];

P-T date friom [A7]

=0.24 => **6457 Pa** at 25oC **SOLID**

Vapor pressure 38.1 mm Hg = **5079 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **38.6**  [A6]*LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 13 | 11.85 | A4 | 49.495 | 49.0 | 49.92 | 0.18 | A2 | 6457 | - | - | - | A4,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**14 Butane**

 Ko=2

lever-arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever-arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-138.2** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **31.779** ± 1.243 **SOLID**

**[A2]:** **P(**25oC**) = 240500 Pa** from P-T dependence from [A7] ***LIQUID***

**[A5]:** **P(**25oC**) =** 1820 mm Hg at 25 deg C = **242606 Pa** ***LIQUID***

ΔHvap(kJ/mol)[25C] **21.02** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 14 | -138.2 | A3 | 31.779 | - | - | 0.50 | A2 | 241551 | 240500 | 242606 | 0.005 | A2,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**15 Diethyl ether**

 Ko=2

lever-arm of the **H3C—CH2-O-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever-arm of the **C-CH2—O-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3) (TWO SUCH BONDS)

??-C?-O?-?? 0.6 [A1]

Melting Temperature(C) **-116.3** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **41.003** ± 0.102 **SOLID**

**[A2]:** **P(**25oC**) = 71142 Pa** from P-T dependence from [A7] ***LIQUID***

Vapor pressure 538 mm Hg = **71715 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **27.1** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 15 | -116.3 | A3 | 41.003 | - | - | 0.04 | A2 | 71578 | 71422 | 71715 | 0.002 | A2,A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**16 Pyridine**

**Rigid** [A1]  **** Ko=2

Melting Temperature(C) **-41.66** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **52.434** ± 1.707 **SOLID**

**[A2]:** **P(**25oC**) = 2722 Pa** from P-T dependence from [A7] ***LIQUID***

Vapor pressure 20.8 mm Hg = **2773 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **40.21** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 16 | -41.66 | A3 | 52.434 | - | - | 0.68 | A2 | 2273 | - | - | 0.0002 | A2,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**17 Pentane**

 Ko=2

lever-arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever-arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-129.7** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **39.974** ± 0.266 **SOLID**

**[A2]:** **P(**25oC**) = 67990 Pa** from P-T dependence from [A7] ***LIQUID***

Vapor pressure 514 mm Hg = **68516 Pa** at 25 deg C [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **26.43** [A6]*LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 17 | -129.7 | A3 | 39.974 | - | - | 0.11 | A2 | 68353 | - | - | 0.004 | A2,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**18 p-benzoquinone** = 1,4-benzoquinone

**Rigid** [A1]  **** Ko=4

Melting Temperature(C) **115.7** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **68.645** from pressure-temperature dependence [A7] (dlnP/dT = ΔHsubl/RT2) **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **66.7 ± 1.6** | kJ/mol | [DSC](http://webbook.nist.gov/chemistry/enthalpy.html#DSC) | [Rojas-Aguilar, Flores-Lara, et al., 2004](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-benzoquinone&Units=SI&cTP=on" \l "ref-2) | AC |
| ΔsubH° | **62.8** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Magnus, 1956](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-benzoquinone&Units=SI&cTP=on#ref-3) | ALS |
| ΔsubH° | **62.760** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Coolidge and Coolidge, 1927](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-benzoquinone&Units=SI&cTP=on#ref-4) | ALS |

ΔHsubl[298K](kJ/mol) = 66.7±1.6 [A9], but see [A13-1] **SOLID**

**[A2]:** Pressure[25C](Pvap)(Pa) **19.576** obtained interpolation from P-T dependence (-4 – 111.6) [A7] **SOLID**

Pressure[25C] 0.1 mm Hg ( 25 °C) = **13.3 Pa** [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 18 | 115.7 | A3 | 65.2 | 62.760 | 68.645 | 1.24 | A2,A7,A9,A13 | 16.1 | 13.3 | 19.576 | 0.44 | A2,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**19 Nitrobenzene**

Ko=2

lever arm of the **ring—NO2** bond: 1.22sin120o=1.06A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **5.7** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **69.49** ± 0.22 **SOLID**

vapor pressure of 0.245 mm Hg at 25 deg C = **32.66 Pa** [A5] ***LIQUID***

ΔHmelt[25C](kJ/mol) 11.59 [A3]

P-T data from [A7]

=0.32 => **44.98 Pa** at 25 oC **SOLID**

ΔHvap(kJ/mol)[25C] **55.01** [A6] ***LIQUID***

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 19 | 5.7 | A3 | 69.49 | 69.27 | 69.71 | 0.09 | A2 | 44.98 | - | - | - | A3,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**20 2-Nitrophenol**

**** Ko=1

lever arm of the **ring—OH** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65

lever arm of the **ring—NO2** bond: 1.22sin120o=1.06A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **44.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 73.25 ± 1.3 [A8, A9] SOLID

73.3 [A8, A9] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **72.30 ± 0.28** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and Gouali, 1994](http://webbook.nist.gov/cgi/cbook.cgi?Name=2-Nitrophenol&Units=SI&cTP=on#ref-5) | Author was aware that data differs from previously reported values; ALS |
| ΔsubH° | **73.3** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and Gouali, 1994, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=2-Nitrophenol&Units=SI&cTP=on#ref-6) | AC |

**Vapor Pressure:** 0.1 MM HG = 13.33 Pa AT 25 DEG C [A14] **SOLID**

0.113 mm Hg at 25 deg C = **15.063** Pa [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 20 | 44.8 | A3 | 72.8 | 72.3 | 73.3 | 0.25 | A9,A13 | 14.17 | 13.33 | 15.063 | 0.06 | A5,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**21 Benzene**

**Rigid** [A1] **** Ko=12

Melting Temperature(C) **5.53** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **44.60** ± 0.20 [A8, A9]

ΔHsubl[25C] = 44.6, 44.8 [A8]; 44.4 [A8, A9] **SOLID**

Vapor pressure for benzene is 94.8 mm Hg = **12637** Pa at 25 deg C [A5] ***LIQUID***

Melting Enthalpy(kJ/mol) **9.95** [A3]

P-T data from [A7]

=0.28 => **16720 Pa** at 25 oC **SOLID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 21 | 5.53 | A3 | 44.6 | 44.4 | 44.8 | 0.04 | A9 | 16720 | - | - | - | A3,A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**22 Phenol**

Ko=2

lever arm of the **ring—OH** bond: 1.0sin109.5o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **40.9** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 69.70 ± 0.90 [A8, A9]

ΔHsubl[25C] = **69.7**± 0.9 [A8, A9] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | 69.7 ± 0.9 | kJ/mol | [ME](http://webbook.nist.gov/chemistry/enthalpy.html#ME) | [Parsons, Rochester, et al., 1971](http://webbook.nist.gov/cgi/cbook.cgi?ID=C108952&Units=SI&Mask=4#ref-7) | AC |
| ΔsubH° | 68.6 | kJ/mol | N/A | [Cox, 1961](http://webbook.nist.gov/cgi/cbook.cgi?ID=C108952&Units=SI&Mask=4#ref-8) | DRB |
| ΔsubH° | 68.66 ± 0.50 | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?ID=C108952&Units=SI&Mask=4#ref-9) | ALS |
| ΔsubH° | 68.7 | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?ID=C108952&Units=SI&Mask=4#ref-9) | DRB |

Vapor pressure 0.35 mm Hg = **46.66 Pa** @ 25 deg C [A5]

*P* (Pa) = 10 @ T0\*=282.8 K, P (Pa) = 100 @ T1\*=307.3  K [A7]  ;

P(25C) = **44.7** Pa **SOLID**

vapor pressure for phenol at 25 °C is 0.3513 mm Hg = **46.83 Pa** [A16] **SOLID**

ΔHvap[25C] (kJ/mol): **57.82** [A6] ***LIQUID***

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 22 | 40.9 | A3 | 68.9 | 68.6 | 69.7 | 0.25 | A9,A13 | 45.77 | 44.7 | 46.83 | 0.02 | A5,A7,A16 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**23 p-Hydroquinone (or 1,4-dihydroxybenzene)**

**** Ko=4

lever arm of the **ring—OH** bond: 1.0sin109.5o=0.94A

K2=1, n2=2 (TWO SUCH BONDS)

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **172.3** [A3]

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **94.13 ± 0.53** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and Buluku, 1991, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on#ref-8) | ΔHfusion =21.09±0.4 kJ/mol; ALS |
| ΔsubH° | **94.1** | kJ/mol | N/A | [Sabbah and Buluku, 1991, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on#ref-8) | DRB |
| ΔsubH° | **94.1 ± 0.5** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and Buluku, 1991, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on#ref-8) | AC |
| ΔsubH° | **99.2 ± 1.7** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Magnus, 1956](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on#ref-9) | Reanalyzed by [Cox and Pilcher, 1970](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on" \l "ref-10), Original value = 104. kJ/mol; ALS |
| ΔsubH° | **103.76** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Coolidge and Coolidge, 1927](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Hydroquinone&Units=SI&cTP=on#ref-11) | ALS |

ΔHsubl[25C]= **94,1** ± 0.5 from [A8, A9] at 25C

Vapor Pressure 0.000019 mm Hg at 25 °C = **0.00253 Pa** [A5, A17] **SOLID** –WHY?

vapour pressure is **0.0024 Pa** (1.8 x 10-5 mmHg) at 25 degrees C [A14] **SOLID** –WHY?

Vapor Pressure: 0.00067 mm Hg @ 25 deg C = **0.089 Pa** [A18] **SOLID** –WHY?

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 23 | 172.3 | A3 | 97.06 | 94.1 | 103.76 | 1.6 | A9,A13 | 0.00818 | 0.0024 | 0.089 | 1.69 | A5,A14,A17,A18 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**24 o-Nitroaniline (or 2-Nitroaniline)**

**** Ko=1

lever arm of the **ring—NO2** bond: 1.22sin120o=1.06A

K2=2, n2=2

**??-A6-N?-?? 10**

lever arm of the **ring—NH2** bond: 1.0sin120o=0.87A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **71.2** [A3]

ΔHsub=**89.0** +-0.7 kJ/mol at 298K [A8, A9] **SOLID**

**Data compiled as indicated in comments:** [*AC*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC) - W.E. Acree, Jr., J.S. Chickos

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | 89.0 ± 0.7 | kJ/mol | [GS](http://webbook.nist.gov/chemistry/enthalpy.html#GS) | [Verevkin, 1997](http://webbook.nist.gov/cgi/cbook.cgi?Name=o-Nitroaniline&Units=SI&cTP=on#ref-2) | AC |

[27] – No info found

vapor pressure at 25 deg C of 2.77X10-3 mm Hg = **0.36 Pa** [A5] **SOLID**

vapor pressure of 8.8X10-4 mm Hg at 25 deg C = **0.12 Pa**  [A19] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 24 | 71.2 | A3 | 89.0 | 88.3 | 89.7 | 0.28 | A9,A13 | 0.21 | 0.12 | 0.36 | 0.55 | A5,A19 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**25 m-Nitroaniline (or 3-Nitroaniline)**

**** Ko=1

lever arm of the **ring—NO2** bond: 1.22sin120o=1.06A

K2=2, n2=2

**??-A6-N?-?? 10**

lever arm of the **ring—NH2** bond: 1.0sin120o=0.87A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **114** [A3]

ΔHsub=**96.5** +-0.3 kJ/mol at 298K [A8, A9] **SOLID**

**Data compiled as indicated in comments:** [*AC*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC) - W.E. Acree, Jr., J.S. Chickos

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **97. ± 1.** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Malaspina, Gigli, et al., 1973](http://webbook.nist.gov/cgi/cbook.cgi?Name=m-Nitroaniline&Units=SI&cTP=on#ref-1) | ALS |
| ΔsubH° | 96.5 ± 0.3 | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Malaspina, Gigli, et al., 1973](http://webbook.nist.gov/cgi/cbook.cgi?Name=m-Nitroaniline&Units=SI&cTP=on#ref-1) | AC see A9 |

[28] – No info found

*P* (Pa) = 0.15 @ T0\*=303 K, P (Pa) = 0.31 @ T1\*=323 K [A20]

 = -0.086;

P(25C)= **0.123** Pa **SOLID** **CONTRADICTION**

vapor pressure at 25 deg C of 9.56X10-5 mm Hg = **0.0127 Pa** [A5, A14] **SOLID**

Vapour Pressure : 3.1E-6 kPa = **0.0031 Pa** (2.3E-5 mmHg)at 25C [A21] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 25 | 114 | A3 | 96.75 | 96 | 98 | 0.31 | A9,A13 | 0.017 | 0.0031 | 0.123 | 1.52 | A5,A19,A20 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**26 p-Nitroaniline (or 4-Nitroaniline)**

**** Ko=2

lever arm of the **ring—NO2** bond: 1.22sin120o=1.06A

K2=2, n2=2

**??-A6-N?-?? 10**

lever arm of the **ring—NH2** bond: 1.0sin120o=0.87A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **146** [A3]

**A2:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **100.8** ± 0.80 (99.3 – 101.5, [A8]) **SOLID**

101.4±1.3; 101.5±1.7; 100.4±2.1; 100.9±.6; 99.3±1.7; 100.7±2.5 [A8, A9] 101.3±0.7 [A9]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **101. ± 1.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 8 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C100016&Units=SI&Type=HSUBLIME) |

vapor pressure of 3.2X10-6 mm Hg at 25 deg C = **0.000427 Pa** at 25 oC [A5] **CONTRADICTION – ERROR!?** **SOLID**

**Vapor Pressure:** 0.0015 mm Hg = 0.2 Pa at 68.0°F =20oC ; 0.007 mm Hg = 0.93 Pa at 86° F = 30oC (NTP, 1992) [A22];

at 25 oC => **0.43** Pa [A22] **SOLID**

vapor pressure at 20 deg C 0.00015 mm Hg = 0.02 Pa [A23]

 = 0.693; = **0.04 Pa** at 25oC **SOLID**

0.2Pa @ 20C [29] – but no info found; [A7] – Too high T

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 26 | 146 | A3 | 101 | 100 | 102 | 0.4 | A9,A13 | 0.015 | 0.000427 | 0.43 | 2.83 | A5,A22,A23 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**27 Aniline**

**** Ko=2

lever arm of the **ring—NH2** bond: 1.0sin120o=0.87A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **-6.02** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **65.245** ± 0.773 **SOLID**

ΔHmelt[25C](kJ/mol) 10.56 [A3]

vapor pressure 0.667 mm Hg = 89.49 Pa [A5] at 25 deg C (*LIQUID*)

=0.49 => **147 Pa** at 25 oC **SOLID**

ΔHvap[25C]: **55.83** [A6] ***LIQUID***

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 27 | -6.02 | A3 | 65.245 | 64.47 | 66.02 | 0.31 | A2 | 147 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**28 Caprolactam (ε-Caprolactam)**

**Rigid** [A1]  **** Ko=2 = 1x2 not flat, chair

Melting point: **69.2 C** [A24] <http://en.wikipedia.org/wiki/Caprolactam>

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 85.300 ± 2.828 (83.3 – ≈87.3 [A8]) SOLID

ΔHsubl = **87.3**±0.2 @ 25C [A8. A9] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | 87.3 ± 0.2 | kJ/mol | N/A | [Kabo, Kozyro, et al., 1992](http://webbook.nist.gov/cgi/cbook.cgi?Name=Caprolactam&Units=SI&cTP=on#ref-5) | AC see [A8,A9] |
| ΔsubH° | **89.76 ± 0.81** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Kabo, Kozyro, et al., 1992, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=Caprolactam&Units=SI&cTP=on#ref-7) | ALS |

vapor pressure 1.9X10-3 mm Hg = **0.25** Pa at 25 deg C [A5, A25] **SOLID**

The vapor pressure of caprolactam is 1.9 × 10-3 mm Hg = **0.25 Pa** at 25 °C [A16] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 28 | 69.2 | A24 | 88.53 | 87.3 | 89.76 | 0.50 | A9,A13 | 0.25 | - | - | - | A5,A16,A25 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**29 Cyclohexane**

…99.99% of all molecules in a cyclohexane solution will be in a chair conformation. [A24]

**Rigid** [A1]  ** ** Ko=24 = 12x2 not flat, chair

Melting Temperature(C) **6.6** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **37.336** ± 0.436 **SOLID**

Melting Enthalpy(kJ/mol) 2.68 [A3]

vapor pressure at 25 deg C 13009 Pa LIQUID [A45] =>

=0.0700 => **13952 Pa** at 25 oC **SOLID**

Pvap[25C]: **12986 Pa** from pressure-temperature dependence (-85.6 - 80.4C [A7]) *LIQUID*

The vapor pressure = 96.9 mm Hg = **12917 Pa** @ 25 deg C [A5] ***LIQUID***

=0.0700 => **13854 Pa** at 25 oC **SOLID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 29 | 6.6 | A3 | 37.336 | 36.9 | 37.772 | 0.17 | A2 | 13902 | 13854 | 13952 | 0.004 | A3,A5,A45 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**30 Hexane**

**** Ko=2

lever arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (THREE SUCH BONDS)

??-C?-C?-?? 1.4[A1]

Melting Temperature(C) **-95.3** [A3]**]**

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **48.571** ± 0. 276 **SOLID**

=298.15; =282.95 LIQUD; =104Pa; =341.45 LIQUD; =105Pa [A7];

 = 0.298;

=**19861 Pa** at 25 oC ***LIQUD***

The vapor pressure = 153mm Hg = **20395 Pa** @ 25 deg C [A5] ***LIQUID***

**ΔHvap(kJ/mol)[25C]** **31.56** from pressure-temperature dependence (-96.4 – 68.3C [A7]) *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 30 | -95.3 | A3 | 48.571 | 48.295 | 48.847 | 0.04 | A2 | 20128 | 19861 | 20395 | 0,013 | A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**31 1h-Benzimidazole**

**Rigid** [A1]  **** Ko=2 – H is not fixed, tautomerism

**Melting Point** 170-172 [A24

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 98.6 ± 3.97 (94.3 – 102.2 [A8]) **SOLID**

ΔHsubl[25C] **= 94.3±0.6**; **102.2±0.4**; **98.9±0.4** [A8, A9]

ΔHvap [kJ/mol] 94.28± 0.6 @ T [K] 298.15 [A10]; but see [A9] SOLID

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **101. ± 7.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 6 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C51172&Units=SI&Type=HSUBLIME) |

vapor pressure of 7.6X10-5 mm Hg at 25 deg C => **0.0101 Pa** [A5, A14] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 31 | 171 | A24 | 99.1 | 94.3 | 102.2 | 1.84 | A8,A9,A13 | 0.0101 | - | - | - | A5,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**32 1h-Indazole**

**Rigid** [A1]  **** Ko=1

Melting point 147-149 [A24]

Refs.[20], [31] do not work;

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **91.0** ± 0.2 [A8] SOLID

ΔHsubl[25C] = **91.1** ± 0.2 [A8, A9] **SOLID**

**Data compiled as indicated in comments:** *[DRB](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB)* - D.R. Burgess

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **91.1 ± 0.2** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Jimenez, Roux, et al., 1987](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-2) | see [Jimenez, Roux, et al., 1986](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-3); ALS |
| ΔsubH° | **91.1** | kJ/mol | N/A | [Jimenez, Roux, et al., 1987](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-2) | DRB |
| ΔsubH° | **91.1 ± 0.2** | kJ/mol | N/A | [Jimenez, Roux, et al., 1987](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-2) | See also [Jimenez, Roux, et al., 1986, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on" \l "ref-4).; AC |
| ΔsubH° | **87.7** | kJ/mol | N/A | [Faour and Akasheh, 1985](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-5) | DRB |
| ΔsubH° | **97.1** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Zimmerman and Geisenfelder, 1961](http://webbook.nist.gov/cgi/cbook.cgi?Name=1h-Indazole&Units=SI&cTP=on#ref-6) | ALS |

Vapour Pressure: 0.0116 mmHg = **1.54 Pa** at 25oC [A26] **SOLID CONTRADICTION**

Vapor Pressure 0.00148 mm Hg at 25oC= **0.197 Pa** [A27] **SOLID CONTRADICTION**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 32 | 148 | A24 | 91.6 | 87.7 | 97.1 | 1.22 | A8,A9,A13 | 0.55 | 0.197 | 1.54 | 0.6 | A26,A27 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**33 p-Nitrotoluene (4-Nitrotoluene)**

**** Ko=2

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6

??-C?-A?-?? 0.1

lever arm of the **ON—ring** bond: 1.22sin118.4o=1.07A

K2=2, n2=2

**??-A6-N?-?? 10** [A1]

Melting Temperature(C) **51.6** [A3]

**A2:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 79.1 ± 2.5 [A8] **SOLID**

79.1, 79.1 ± 2.5 [A8, A9]; 74.8±1.0 [A9] see [A13] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **74.8 ± 1.0** | kJ/mol | [GS](http://webbook.nist.gov/chemistry/enthalpy.html#GS) | [Widegren and Bruno, 2010](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Nitrotoluene&Units=SI&cTP=on#ref-2) | AC |
| ΔsubH° | **79. ± 3.** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Lenchitz, Velicky, et al., 1971](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Nitrotoluene&Units=SI&cTP=on#ref-3) | ALS |
| ΔsubH° | **79.1 ± 2.5** | kJ/mol | [ME](http://webbook.nist.gov/chemistry/enthalpy.html#ME) | [Lenchitz, Velicky, et al., 1971](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Nitrotoluene&Units=SI&cTP=on#ref-3) | AC |
| ΔsubH° | **79.1** | kJ/mol | N/A | [Lenchitz and Velicky, 1970](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Nitrotoluene&Units=SI&cTP=on#ref-4) | AC |

vapor pressure of 0.164 mm Hg at 25 deg = **21.86 Pa** [A28] **CONTRADICTION – ERROR!? SOLID**

0.0157 mm Hg = **2.09 Pa** at 25 deg C /extrapolated/ [A5] **CONTRADICTION – ERROR!? SOLID**

*P* (Pa) = 5.11 @ T0\*=303 K, P (Pa) = 30.47 @ T1\*=323 K [A20]

 = -0.209;

P(25C)=**3.16 Pa** **CONTRADICTION – ERROR!? SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 33 | 51.6 | A3 | 78 | 74.8 | 79.1 | 1.09 | A8,A9,A13 | 5.2 | 2.09 | 21.86 | 1.09 | A5,A20,A28 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**34 Toluene**

**** Ko=2

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6

??-C?-A?-?? 0.1 [A1]

Melting Temperature(C) **-95** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **46.34** ± 4.75 SOLID *(LIQUD)*

ΔHsubl[25C]= **43.1** [A8, A9] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **43.1** | kJ/mol | [B](http://webbook.nist.gov/chemistry/enthalpy.html#B) | [Lenchitz and Velicky, 1970](http://webbook.nist.gov/cgi/cbook.cgi?Name=Toluene&Units=SI&cTP=on#ref-10) | AC see [A8,A9] |

vapor pressure for toluene at 25 °C is 28.4 mm Hg = **3786 Pa** at 25 oC [A5, A29] ***LIQUID***

ΔHvap(kJ/mol)[25C] **38.01** [A6] *LIQUID*

[A6] CRC Handbook of Chemistry and Physics by David R. Lide (Editor),78-th edition, CRC-press Inc. Enthalpy of vaporization 6-105{6-115 p.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 34 | -95 | A3 | 43.1 | - | - | - | A8,A9,A13 | 3786 | - | - | - | A5,A29 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**35 o-Cresol (**2-methylphenol; 2-hydroxytoluene**)**

**** Ko=1

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6

??-C?-A?-?? 0.1

lever arm of the **HO—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **29.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **75.40** ± 0.85 (74.8, 76.0±0.8, 288K [A8]) SOLID

**74.8**, 76.0±0.8, 288K [A8, A9]; **73.7±0.5**, 298K [A9], but see [A13] SOLID

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **73.7 ± 0.5** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Richard, Bernardes, et al., 2007](http://webbook.nist.gov/cgi/cbook.cgi?Name=o-Cresol&Units=SI&cTP=on#ref-7) | AC |
| ΔsubH° | **76.0** | kJ/mol | N/A | [Cox, 1961](http://webbook.nist.gov/cgi/cbook.cgi?Name=o-Cresol&Units=SI&cTP=on#ref-8) | DRB |
| ΔsubH° | **76.02 ± 0.75** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=o-Cresol&Units=SI&cTP=on#ref-9) | ALS |
| ΔsubH° | **76.0** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=o-Cresol&Units=SI&cTP=on#ref-9) | DRB |

vapor pressures, at 25°C, *o*-cresol, 0.299 mm Hg = **39.9 Pa** [A5, A30] **SOLID**

vapor pressures, at 20°C, *o*-cresol, 0.3 mm Hg = **40.0 Pa** [A13] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 35 | 29.8 | A3 | 75.4 | 73.7 | 76.02 | 0.39 | A9,A13 | 39.95 | 39.9 | 40.0 | 0.001 | A5,A13,A30 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**36 p-Cresol (**4-methylphenol; 4-Cresol; 4-Hydroxytoluene**)**

**** Ko=2

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6

??-C?-A?-?? 0.1

lever arm of the **HO—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **35.5** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **73.90** ± 1.50, 290K [A8] SOLID

73.90 ± 1.50, 290K; [A8, A9]; 73.1±0.6, 298K [A9]; but see [A13] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **73.1 ± 0.6** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Richard, Bernardes, et al., 2007](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Cresol&Units=SI&cTP=on#ref-7) | AC |
| ΔsubH° | **73.9** | kJ/mol | N/A | [Cox, 1961](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Cresol&Units=SI&cTP=on#ref-8) | DRB |
| ΔsubH° | **73.9 ± 1.5** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Cresol&Units=SI&cTP=on#ref-9) | ALS |
| ΔsubH° | **73.9** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=p-Cresol&Units=SI&cTP=on#ref-9) | DRB |

vapor pressures, at 25 °C, *p*-cresol, 0.11 mm Hg = **14.6 Pa** [A5, A30] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 36 | 35.5 | A3 | 73.7 | 73.1 | 73.9 | 0.36 | A9,A13 | 14.6 | - | - | - | A5,A30 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**37 Heptane**

 Ko=2

lever arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (FOUR SUCH BONDS)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-90.6** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **56.125** ± 0.418 from P-T dependence from [A7] **SOLID**

=298.15; =266.55 LIQUD; =103Pa; =308.55 LIQUD; =104Pa [A7]

 = 0.779;

=6012 Pa at 25oC *LIQUD*

Vapor Pressure: 46 mm Hg @ 25 deg C = **6132 Pa** [A5, A31] ***LIQUD***

ΔHvap(kJ/mol)[25C] **36.57** [A6] *LIQUD*

[A6] CRC Handbook of Chemistry and Physics by David R. Lide (Editor),78-th edition, CRC-press Inc. Enthalpy of vaporization 6-105{6-115 p.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 37 | -90.6 | A3 | 54.125 | - | - | 0.418 | A2,A7 | 6132 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**38 Acetophenone**

**** Ko=2

lever arm of the **ring—CO-C** bond: (1.389+1.09)sin120o=2.15A

K1=1, n1=2

??-C?-A?-?? 0.1

lever arm of the **ring-C—CH3** bond: 1.09sin109.5o=1.03A

K2=3, n2=3

**??-C?-A?-?? 0.1** [A1]

Melting Temperature(C) **20.5 [A32]**

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **71.076** ± 2.17 **SOLID**

Enthalpy of fusion (kJ/mol) 14.16 [A3] =2.47866 kJ/mo

1) Vapor Pressure 0.44 mm Hg at 25 oC = **58.7** Pa [A32] *LIQUID*

2) Vapor Pressure 0.397 mm Hg at 25 oC = **52.9** Pa [A5] *LIQUID*

1) =0.09 => **57.9 Pa** at 25 oC **SOLID**

2) =0.09 => **64.2 Pa** at 25 oC **SOLID**

ΔHvap(kJ/mol)[25C] **57.849** obtained from extrapolation of pressure-temperature dependence (36 - 201.5C) *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 38 | 20.5 | A32 | 71.076 | - | - | 0.87 | A2 | 61.0 | 57.9 | 64.2 | 0.05 | A3,A5,A32 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**39 p-Xylene**

**** Ko=4

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1 [A1]

Melting Temperature(C) **13.25** [A4]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **59.936** ± 0.072 **SOLID**

Melting Enthalpy(kJ/mol) 17.12 [A4][

Pvap[25C] = 8.84 mm Hg =**1178** Pa at 25oC [A5, A10] *LIQUID*

 = .28 **1565 Pa** at 25 C **SOLID**

ΔHvap(kJ/mol)[25C] **42.4** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 39 | 13.25 | A4 | 59.936 | - | - | 0.072 | A2 | 1565 | - | - | - | A4,A5,A10 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**40 2,3-Xylenol =** 2,3-dimethylphenol

 Ko=1

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1

lever arm of the **OH—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **72.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **84.0** ± 1.0 (from T=283–323K of [A8], [A9]) **SOLID**

**Data compiled as indicated in comments:** *[DRB](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB)* - D.R. Burgess

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **84.0 ± 1.0** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C3-Xylenol&Units=SI&cTP=on#ref-2) | ALS |
| ΔsubH° | **84.0** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C3-Xylenol&Units=SI&cTP=on#ref-2) | DRB |
| ~~Δ~~~~sub~~~~H°~~ | ~~59.4 ± 0.8~~ | ~~kJ/mol~~ | [~~V~~](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [~~Wolf and Weghofer, 1938~~](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C3-Xylenol&Units=SI&cTP=on#ref-3) | ~~ALS~~ was not even considered  by Chickos &Acree {A8,A9] |

Vapor pressure[25C], Pvap(Pa)= **3.49** by interpolation of the P-T dependence (14.3 – 57.2C, [A4]) **SOLID**

Vapor pressure at 25 deg C  of 0.089 mm Hg = **11.86 Pa** [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 40 | 72.8 | A3 | 84.0 | 84.0 | 84.0 | 0.28 | A2,A8,A9,A13 | 6.42 | 3.49 | 11.86 | 0.61 | A4,A10 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**41 2,5-Xylenol =** 2,5-dimethylphenol

 Ko=1

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1

lever arm of the **OH—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **74.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 85.0± 0.25 [A8] [A9] SOLID

282–323K **85.0** +-0.25 [A9] but see [A13] SOLID

**Data compiled as indicated in comments:** *[DRB](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB)* - D.R. Burgess

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **85.0 ± 0.3** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C5-Xylenol&Units=SI&cTP=on#ref-3) | ALS |
| ΔsubH° | **84.6** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C5-Xylenol&Units=SI&cTP=on#ref-3) | DRB |

Pressure[25C](Pvap)(Pa) **3.929** obtained extrapolation from P-T dependence (13.4 – 55.9C [A7]) **SOLID**

vapor pressure at 25 deg C of 0.156 mm Hg = **20.8 Pa** [A5, A14] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 41 | 74.8 | A3 | 84.8 | 84.6 | 85.0 | 0.11 | A9,A13 | 9.02 | 3.929 | 20.8 | 0.83 | A7,A5,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**42 2,6-Xylenol = 2,6-dimethylphenol**

 Ko=2

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1

lever arm of the **OH—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **45.7** [A3]

[A2]: ΔHsubl[25C] ≡ -ΔHcryst[25C] **75.6**±1.0 [A8] SOLID

277–323K **75.6** ±0.17 (277–313) [A8]; **75.6,** but see [A13]-1]**, 75.1** [A9] (298) **SOLID**

Note: Last author refers to the determined value as the enthalpy of vaporization even though the compound is a solid

ΔHsubl[298K](kJ/mol) = **75.31** [A6] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **75.6** | kJ/mol | N/A | [Morawetz, 1971](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C6-Xylenol&Units=SI&cTP=on#ref-3) | AC |
| ΔsubH° | **75.1** | kJ/mol | N/A | [Morawetz, Elvebredd, et al., 1968](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C6-Xylenol&Units=SI&cTP=on#ref-4) | Author of {R1968MOR/ELV1509-1531} refers to the determined value as the enthalpy of vaporization even though the compound is a solid; AC |
| ΔsubH° | **75.6 ± 0.2** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C6-Xylenol&Units=SI&cTP=on#ref-5) | ALS |
| ΔsubH° | **75.6** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C6-Xylenol&Units=SI&cTP=on#ref-5) | DRB |
| ~~Δ~~~~sub~~~~H°~~ | ~~59.4 ± 0.8~~ | ~~kJ/mol~~ | [~~V~~](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [~~Wolf and Weghofer, 1938~~](http://webbook.nist.gov/cgi/cbook.cgi?Name=2%2C6-Xylenol&Units=SI&cTP=on#ref-6) | ~~ALS~~ was not even considered by Chickos &Acree {A8,A9] |

Pressure[25C](Pvap)(Pa) **23.624** obtained extrapolation from P-T dependence (-3.1 – 39.6C [A2,A7]) **SOLID**

vapor pressure at 25 deg C  of 0.274 mm Hg = **36.5 Pa** [A5, A14] **SOLID**

T=25C ΔHvap=**75.31** kJ/mol [A6] *LIQUD*

**Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 42 | 45.7 | A3 | 75.44 | 75.1 | 75.6 | 0.10 | A6,A9,A13 | 29.4 | 23.624 | 36.5 | 0.22 | A2,A7,A5,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**43 3,4-Xylenol = 3,4-dimethylphenol**

 Ko=1

lever arm of the **H3C—ring** bond: 1.09sin109.5o=1.03A

K1=3, n1=6 (TWO SUCH BONDS)

??-C?-A?-?? 0.1

lever arm of the **OH—ring** bond: 1.0sin110o=0.94A

K2=1, n2=2

??-A?-OH-?? 1.65 [A1]

Melting Temperature(C) **60.8** [A3]

**A2:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 85.7 ± 0.1 [A8], [A9] 282–323K SOLID

[A8] 282–323K **85.1** (but see [A13}-1)**, 85.0** [A9] 298 (but see [A13}-2) **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **85.1** | kJ/mol | N/A | [Morawetz, 1971](http://webbook.nist.gov/cgi/cbook.cgi?Name=3%2C4-Xylenol&Units=SI&cTP=on#ref-4) | AC |
| ~~Δ~~~~sub~~~~H°~~ | ~~85.0~~ | ~~kJ/mol~~ | ~~N/A~~ | [~~Morawetz, Elvebredd, et al., 1968~~](http://webbook.nist.gov/cgi/cbook.cgi?Name=3%2C4-Xylenol&Units=SI&cTP=on#ref-5) | ~~Author of {R1968MOR/ELV1509-1531} refers to the determined value as the enthalpy of vaporization even though the compound is a solid; AC~~ |
| ΔsubH° | **85.7 ± 0.1** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=3%2C4-Xylenol&Units=SI&cTP=on#ref-6) | ALS |
| ΔsubH° | **85.8** | kJ/mol | N/A | [Andon, Biddiscombe, et al., 1960](http://webbook.nist.gov/cgi/cbook.cgi?Name=3%2C4-Xylenol&Units=SI&cTP=on#ref-6) | DRB |

Pressure[25C](Pvap)(Pa) **1.8358** obtained extrapolation from P-T dependence (19.7 – 63.7C [A2,A7]) **SOLID**

vapor pressure at 25 deg C of 0.036 mm Hg = **4.78 Pa** [A5, A14] **SOLID**

T=25C ΔHvap=**85.03** kJ/mol=20.32kcal/mol [A6] *LIQUD*

**Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 43 | 60.8 | A3 | 85.4 | 85.0 | 85.8 | 0.14 | A9,A13 | 2.96 | 1.8358 | 4.78 | 0.48 | A2,A5,A7,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**44 Octane**

 Ko=2

lever arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (FIVE SUCH BONDS)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-56.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **66.366** ± 0.127 **SOLID**

vapor pressure at 25 deg C of 14.1 mm Hg = **1880 Pa** [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **41.49** [A6] *LIQUID*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 44 | -56.8 | A3 | 66.366 | - | - | 0.05 | A2 | 1880 | - | - | - | A5 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**45 Isoquinoline**

**Rigid** [A1]  **** Ko=1

Melting Temperature(C) **26.47** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **80.397** ± 0.102 with ΔHvap(kJ/mol)=67.061 from P-T dependence with data from [A7]  **SOLID**

ΔHmelt(kJ/mol)=**13.54** [A9], [A3], [A13]; ΔHmelt(kJ/mol)[at triple point, 299.62K=26.47oC]=**13.544** [A33],

ΔHvap(kJ/mol) [at triple point, 299.62K=26.47oC]=**60.3**± 1.0 [A33],

ΔHvap(kJ/mol) at 25C =**60.26** [A6] *LIQUID*

ΔHvap(kJ/mol) at 25C =**67.061 -** from P-T dependence with data from [A2,A7] (>30.2oC)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***ONLY LIQUID*** [A13]: ΔvapH° | **59.5** | kJ/mol | N/A | [Steele, Archer, et al., 1988, 2](http://webbook.nist.gov/cgi/cbook.cgi?ID=C119653&Units=SI&Mask=4#ref-3) |
| ***ONLY LIQUID*** [A13]: ΔfusH°=13.54 | | T=299.6 | [Domalski and Hearing, 1996](http://webbook.nist.gov/cgi/cbook.cgi?ID=C119653&Units=SI&Mask=4#ref-8) | |

ΔHsubl[T=25C] = ΔHmelt(Tmelt) + (T-Tmelt)(Cp,liq - Cp,cryst) + ΔHvap(T) = **13.54 - (-1.47)\*0.025 + 60.26 = 73.84 kJ/mo**± 1.0  **SOLID**

ΔHsubl(kJ/mol) [at triple point, 299.62K=26.47oC]=**73.844**± 1.0 [A33],  **SOLID**

Pressure [25C], Pvap= **6.226 Pa** obtained from P-T dependence (30,2 – 242.7C, [A2,A7]) *LIQUID*

 = -0.027 => **6.06 Pa** at 25oC **SOLID**

Pressure [triple point, 299.62K=26.47oC , Pvap)= **9.53 Pa** [A33] 26.47oC, *LIQUID/SOLID*

 =-0.030 =>**9.25 Pa** at 25oC **SOLID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 45 | 26.47 | A3 | 77.12 | 73.84 | 80.397 | 1.3 | A2,A3,A6,A7,A9,A33 | 7.49 | 6.06 | 9.25 | 0.21 | A2,A7,A33 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**46 Nonane**

 Ko=2

lever arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

K1=3, n1=3 (TWO SUCH BONDS)

??-C?-C?-?? 1.4

lever arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (SIX SUCH BONDS)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-53.5** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **65.638** ± 0.100 **SOLID**

ΔHsubl[25C] **71.4** [A8] **SOLID**

Pressure[25C](Pvap)(Pa) **573.8** obtained from P-T dependence [A7] ***LIQUD***

vapor pressure at 25 deg C of 4.45 mm Hg = **593 Pa** [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] 46.595 obtained from interpolation of pressure-temperature dependence (-46.8 - 150.5C [A2,A7]) *LIQUD*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Comment** |
| ΔvapH° | 46.5 ± 0.2 | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | [A5], ***LIQUD*** |

ΔHvap(kJ/mol)[25C] 46.41 [A6]*LIQUD*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 46 | -53.5 | A3 | 68.5 | 65.638 | 71.4 | 0.8 | A2,A8 | 583 | 573.6 | 593 | 0.02 | A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**47 Naphthalene**

**Rigid** [A1]  **** Ko=4

Melting Temperature(C) **80.2** [A3]

**A2:** ΔHsubl[25C] ≡ -ΔHcryst[25C] 72.186 ± 0. 836 (70.4 – 73.0, [A8, A9] – after 1970) **SOLID**

[A8, A9] – after 1970 **70.4, 72.3±0.4, 72.6±0.1, 72.4±0.7, 72.5, 72.1±0.25, 73.0±0.3** **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **71. ± 5**. | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 17 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C91203&Units=SI&Type=HSUBLIME) |

=298.15; =297.25 SOLID; =10Pa; =322.45 SOLID; =102Pa [A7];

 = 0.039;

=**10.9** Pa at 25 oC from P-T dependence (data from [A7] **SOLID**

vapor pressure at 25 deg C of 0.085 mm Hg = **11.3 Pa** [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 47 | 80.2 | A3 | 72.0 | 70.4 | 73.0 | 0.8 | A8,A9,A13 | 11.1 | 10.9 | 11.3 | 0.02 | A5,A7,A14 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**48 Decane**

 Ko=2

lever arm of the **H3C—CH2-C-** bond: 1.09sin109.5o=1.03A

??-C?-C?-?? 1.4

K1=3, n1=3 (TWO SUCH BONDS)

lever arm of the **C-CH2—CH2-C** bond: 1.525 sin109.5o=1.44A

K2=1, n2=3 (SEVEN SUCH BONDS)

??-C?-C?-?? 1.4 [A1]

Melting Temperature(C) **-29.7** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **83.887** ± 0. 929 **SOLID**

ΔHsubl[25C] **82.4** [A8] **SOLID**

Pressure[25C](Pvap)(Pa) **180.91** obtained from interpolation of P-T dependence [A7] ***LIQUD***

vapor pressure at 25 deg C of 1.43 mm Hg = **191 Pa** [A5] ***LIQUID***

ΔHvap(kJ/mol)[25C] **51.376** obtained from interpolation of pressure-temperature dependence (-10.6 – 173.7C, [A2,A7]) *LIQUD*

ΔHvap(kJ/mol)[25C] **51.42** [A6] *LIQUD*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 48 | -29.7 | A3 | 83.1 | 82.4 | 88.887 | 0.31 | A2,A8 | 186 | 180.91 | 191 | 0.03 | A5,A7 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**49 Dibenzofuran**

**Rigid** [A1]  **** Ko=2 - flat

[Melting point](http://en.wikipedia.org/wiki/Melting_point" \o "Melting point) 81 - 85°C [A24]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **80.45** ± 5.58 (76.5 – 84.4 [A8, A9]) SOLID

[A9] **82.0±0.2** , **84.4±0.7**, **76.5±0.2** **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **81. ~~± 9.~~** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 6 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C132649&Units=SI&Type=HSUBLIME) TOO big error not supported by other data – see below - **IGNORE** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **ΔsubH (kJ/mol)** | **Temperature (K)** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| 82.1 ± 1.5 | 295. - 318. | [ME](http://webbook.nist.gov/chemistry/enthalpy.html#ME) | [Li, Shibata, et al., 2004](http://webbook.nist.gov/cgi/cbook.cgi?ID=C132649&Units=SI&Mask=4#ref-8) | AC |

0.00248 mm Hg = **0.33 Pa** @ 25 deg C [A5] (as was in [20]) **SOLID**

0.0175 mm Hg at 25 °C = 2.33 Pa [A34] **SOLID**

[20]. [33] – no data now

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 49 | 83 | A24 | 81.0 | 76.5 | 84.4 | 1.2 | A9,A13 | 0.88 | 0.33 | 2.33 | 0.98 | A5,A34 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**50 Dibenzothiophene**

**Rigid** [A1]  **** Ko=2 - flat

Melting Temperature(C) 97 – 100 [A24]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **85.1** ± 0.4 [A8] SOLID

**93.2**±0.5 (2009FRE/GOM); **85.1**±0.4 (1979SAB); **97.5** (2009FRE/GOM) [A9] **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **90. ~~± 10~~.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 6 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C132650&Units=SI&Type=HSUBLIME) TOO big error not supported by other data – see below - **IGNORE** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **ΔsubH (kJ/mol)** | **Temperature (K)** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| 91.2 | 303. - 348. | [T](http://webbook.nist.gov/chemistry/enthalpy.html#T) | [Hansen and Eckert, 1986](http://webbook.nist.gov/cgi/cbook.cgi?ID=C132650&Units=SI&Mask=4#ref-10) | AC |
| 90.7 | 333. - 363. | [GS](http://webbook.nist.gov/chemistry/enthalpy.html#GS) | [Edwards and Prausnitz, 1981](http://webbook.nist.gov/cgi/cbook.cgi?ID=C132650&Units=SI&Mask=4#ref-9) | AC |

[21] is not available now – no data for P

Vapor pressure @ 20-25 degC (mmHG) 2.046934913e-005 = **0.00273 Pa** [A35] **SOLID**

extrapolated vapor pressure at 25 deg C: 2.05X10-4 mm Hg = **0.0273 Pa** [A14] **SOLID**

VP (Pa, 25 deg C): **0.00912** (Modified Grain method) [A36] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 50 | 98.5 | A24 | 91.5 | 85.1 | 97.5 | 1.8 | A9,A13 | 0.0086 | 0.00273 | 0.0273 | 0.97 | A14,A35,A36 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**51 Carbazole**

**Rigid** [A1]  **** Ko=2 – flat

Melting Temperature(C) **246.2** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **100.5** ± 3.96 <**97.7±0.3**, **103.3±1.1** [A8], [A9]]> **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **102~~. ± 8.~~** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 7 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C86748&Units=SI&Type=HSUBLIME) TOO big error not supported by other data – see below - **IGNORE** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **ΔsubH (kJ/mol)** | **Temperature (K)** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| 101.2 ± 1.1 | 346. - 364. | [ME](http://webbook.nist.gov/chemistry/enthalpy.html#ME) | [Jimenez, Roux, et al., 1990](http://webbook.nist.gov/cgi/cbook.cgi?Name=Carbazole&Units=SI&cTP=on#ref-7) | AC |

vapor pressure of 1.37X10-6 mm Hg at 25 deg C = **0.000183 Pa – appr**. [A5, A14] **SOLID** **CONTRADICTION?**

Vapor pressure @ 20-25 degC (mmHG) 0.000266 **0.0355 Pa – appr** [A35] **SOLID ERROR?**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 51 | 246.2 | A3 | 101.0 | 97.7 | 103.2 | 1.07 | A8,A9,A13 | 0.00255 | 0.000183 | 0.0355 | 2.63 | A5,A14,A35 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**52 10H-Phenothiazine (Phenothiazine)**

**Rigid** [A1]  ****Ko=4 - not flat

Melting Temperature(C)185 °C [A24] <http://en.wikipedia.org/wiki/Phenothiazine>

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **85 ± 1.4** ([A8] and P-T dependence from [37] ; seems to be wrong now

**114.5**± 0.4for 298K [A9]; – WHY such a difference in ΔHsubl??? (see [A13]) **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **111.45 ± 0.37** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and El Watik, 1992](http://webbook.nist.gov/cgi/cbook.cgi?Name=10H-Phenothiazine&Units=SI&cTP=on#ref-5) | ALS |
| ΔsubH° | **114.5 ± 0.4** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Sabbah and El Watik, 1992](http://webbook.nist.gov/cgi/cbook.cgi?Name=10H-Phenothiazine&Units=SI&cTP=on#ref-5) | AC |

Vapor Pressure: 1.06E-05 mmHg at 25°C = **0.00140** Pa [A37] ]+many others **SOLID**

estimated vapor pressure of 8.9X10-7 mm Hg = **0.00012** Pa at 25 deg [A13]+many others **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 52 | 185 | A24 | 112.95 | 111.45 | 114.45 | 0.60 | A9,A13 | 0.00041 | 0.00012 | 0.00140 | 1.07 | A13,A47 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**53 Acenaphthene**

**Rigid** [A1]  **** Ko=2 - flat

Melting Temperature(C) **93.4** [A3]

**A2:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **84.22** ± 1.99(83.4 – 84.6 [A8], [A9]; see [A13] ) **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **84.8 ± 0.4** | kJ/mol | [Review](http://webbook.nist.gov/chemistry/enthalpy.html#Review) | [Roux, Temprado, et al., 2008](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on#ref-12) | There are sufficient high-quality literature values to make a good evaluation with a high degree of confidence. In general, the evaluated uncertainty limits are on the order of (0.5 to 2.5) kJ/mol.; DRB |
| ΔsubH° | **84.6** | kJ/mol | [CGC-DSC](http://webbook.nist.gov/chemistry/enthalpy.html#CGC-DSC) | [Chickos, Hesse, et al., 1998](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on#ref-8) | AC |
| ΔsubH° | **83.4 ± 1.0** | kJ/mol | N/A | [Osborn and Douslin, 1975, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on#ref-13) | See also [Finke, Messerly, et al., 1977, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on" \l "ref-14).; AC |
| ΔsubH° | **86. ± 1.** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Boyd, Christensen, et al., 1965](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on#ref-15) | ALS |
| ΔsubH° | **86.0** | kJ/mol | N/A | [Boyd, Christensen, et al., 1965](http://webbook.nist.gov/cgi/cbook.cgi?Name=Acenaphthene&Units=SI&cTP=on#ref-15) | DRB |

Vapour pressure, Pa at 25°C: **0.3 Pa** [A5]  **SOLID**

vapor pressure of 2.5X10-3 mm Hg at 25 deg C **= 0.3333 Pa** [A38] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 53 | 93.4 | A3 | 85. | 83.4 | 86.0 | 0.49 | A8,A9,A13 | 0.316 | 0.3 | 0.3333 | 0.05 | A5,A38 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**54 Biphenyl (Diphenyl)**

; Ko=4

lever arm of the **ring— ring** bond: (1.389+1.09)sin120o=2.15A

K1=2, n1=2

**A6-A6-A6-A6 20** [A1]

Melting Temperature(C) **69** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **80.16** ± 3.01 **(77.9 --- 82.9 [A8], [A9] ) SOLID**

**82.9**; **81.5 ± 0.2**; **77.9 ± 0.3**; **81.8 ± 0.2**; **81.8 ± 0.4** [A8, A9]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **82. ± 3.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 10 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C92524&Units=SI&Type=HSUBLIME) |

vapor pressure of biphenyl is 0.01 mm Hg at 25 °C = **1.333 Pa** [A39]  **SOLID**

8.93X10-3 mm Hg at 25 deg C == **1.19** Pa at 25°C [A5] **SOLID**

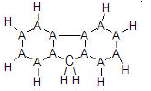
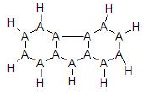
**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 54 | 69 | A3 | 81.3 | 77.9 | 82.9 | 0.81 | A8,A9,A13 | 1.26 | 1.19 | 1.333 | 0.06 | A5,A39 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**55 Fluorene (9H-Fluorene)**

**Rigid** [A1]  **** Ko=2 – flat

**, not  ~~~~ !!!**

Melting Temperature(C) **114.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **85.66** ± 3.29 [A8], [A9]

**87.6**; **85.1** ± 0.4; **80.2** ± 0.2 [A8, A9]; **86.1** ± 0.6 [A9] **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| ΔsubH° | **84. ± 5.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 9 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C86737&Units=SI&Type=HSUBLIME) |

Vapor pressure **0.0658 Pa** at 25 deg C [A40]  **SOLID**

Vapor pressure = 3.2X10-4 mm Hg **= 0.043 Pa** at 20 deg C [A5]  **SOLID**

Vapor pressure @ 20-25 degC (mmHG) 0.0032404409009 ~~torr~~ **= 0.432 Pa** [A35] **SOLID** **CONTRADICTION**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 55 | 114.4 | A3 | 84.6 | 80.2 | 87.6 | 1.3 | A8,A9,A13 | 0.136 | 0.043 | 0.432 | 1.1 | A5,A35,A40 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**56 Anthracene**

**Rigid** [A1]  **** Ko=4

Melting Temperature(C) **215** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **102.27** ± 2.61 [A8] [A9] **SOLID**

**99.4**; **104.5** ± 1.5; **102.9** ± 4.8; **84** ± 3 [A8, A9]; **98.2**; **100.2** ± 0.4; **96.3**± 0.7; [A9]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13]: ΔsubH° | **98. ± 10.** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 12 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C120127&Units=SI&Type=HSUBLIME) |

6.56X10-6 mm Hg at 25 deg C (exptrapolated) = **0.00087** Pa [A5] **SOLID CONTRADICTION**

Vapour pressure, Pa at 25°C: **0.08** Pa [A5] **SOLID CONTRADICTION**

Vapour pressure, Pa at 25°C: **0.08** Pa [A21] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 56 | 215 | A3 | 97.9 | 84 | 104.5 | 2.9 | A8,A9,A13 | 0.0083 | 0.00087 | 0.08 | 2.26 | A5,A21 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**57 Phenanthrene**

**Rigid** [A1]  **** Ko=2

Melting Temperature(C) **99.24** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **89.80** ± 2.28

**90.5**; **90.9** ± 1.7; **92.5** ± 2.0; **87.4** ± 0.8; **86.6** ± 0.8; **90.9** ± 0.4 [A8, A9]; **89.6** ± 0.8; **92.5** ± 0.4 [A9] **SOLID**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13]: ΔsubH° | **91. ± 3**. | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 12 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C85018&Units=SI&Type=HSUBLIME) |

Vapor pressure @ 20-25 degC (mmHG) 0.00068 **= 0.091 Pa** [A35] **SOLID**

vapor pressure of 1.21X10-4 mm Hg at 25 deg C**= 0.0161 Pa** [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 57 | 99.24 | A3 | 90.3 | 86.6 | 92.5 | 0.98 | A8,A9,A13 | 0.038 | 0,0161 | 0.091 | 0.87 | A5,A35 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **solubility** | 57 | Phenanthrene | 0.001071 | g/L, 25C | 0.00000601 | C (mol/L) | log[C(mol/L)] | -5.22 | [A5],[B1] - mean geom. |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**58 trans-Stilbene (trans 1,2-diphenylethene)**

****  Ko=2

lever arm of the **ring—CH-CH** bond: (1.389+1.09)sin120o=2.15A

K1=2, n1=2 (TWO SUCH BONDS)

**??-A?-A?-?? 10**

lever arm of the **ring-CH—CH-ring** bond: (1.09+.6845+1.389+.6845+1.389)sin120o=5.26A

K2=1, n2=2

**??-A?-A?-?? 10** [A1]

Melting Temperature(C) **123** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **100.77** ± 1.20 [A8, A9] **SOLID**

**102**; **100.7** ± 0.4: **99.6** ± 1.7 [A8, A9]; **102** ± 0.4 [A9]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13]: ΔsubH° | **98. ~~± 10.~~** | kJ/mol | [AVG](http://webbook.nist.gov/chemistry/site-cal.html#AVG) | N/A | Average of 6 values; [Individual data points](http://webbook.nist.gov/cgi/cbook.cgi?ID=C103300&Units=SI&Type=HSUBLIME); TOO big error not supported by other data – see below. IGNORE |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **ΔsubH (kJ/mol)** | **Temperature (K)** | **Method** | **Reference** | **Comment** |
| 99.6 | 298. - 343. | [A](http://webbook.nist.gov/chemistry/enthalpy.html#A) | [Stephenson and Malanowski, 1987](http://webbook.nist.gov/cgi/cbook.cgi?Name=trans-Stilbene+&Units=SI&cTP=on#ref-8) | AC |
| 103.8 ± 2.5 | 293. - 338. | N/A | [Kratt, Beckhaus, et al., 1983](http://webbook.nist.gov/cgi/cbook.cgi?Name=trans-Stilbene+&Units=SI&cTP=on#ref-9) | AC |

vapor pressure of 8.81X10-4 mm Hg at 25 deg C **= 0.1173 Pa** [A5, A41] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 58 | 123 | A3 | 100.5 | 98 | 102 | 1.9 | A8,A9,A13 | 0.1173 | - | - | - | A5,A41 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**59 Fluoranthene**

**Rigid** [A1]  **** Ko=2 - flat

Melting Temperature(C) **~~111~~ 107.8** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **91.90** ± 10.3 <averaged over T=25C, 30C> – WHY **30C**?

Temperature(C) \_Hsub(kJ/mol) Reference

25 **99.2±0.8** [A8, A9] **SOLID**

**Data compiled as indicated in comments:** *[DRB](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB)* - D.R. Burgess

*[ALS](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS)* - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13]: ΔsubH° | **101.2 ± 2.8** | kJ/mol | [Review](http://webbook.nist.gov/chemistry/enthalpy.html#Review) | [Roux, Temprado, et al., 2008](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on#ref-6) | There are sufficient high-quality literature values to make a good evaluation with a high degree of confidence. In general, the evaluated uncertainty limits are on the order of (2 to 4) kJ/mol.; *DRB* |
| [A13]: ΔsubH° | **99.2 ± 0.8** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Morawetz, 1972](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on#ref-7) | ALS |
| [A13]: ΔsubH° | **99.2 ± 0.8** | kJ/mol | [C](http://webbook.nist.gov/chemistry/enthalpy.html#C) | [Morawetz, 1972, 2](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on#ref-8) | See also [Pedley and Rylance, 1977](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on" \l "ref-9).; AC |
| [A13]: ΔsubH° | **102. ± 2.** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Boyd, Christensen, et al., 1965](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on#ref-10) | ALS |
| [A13]: ΔsubH° | **100.0** | kJ/mol | N/A | [Boyd, Christensen, et al., 1965](http://webbook.nist.gov/cgi/cbook.cgi?Name=Fluoranthene&Units=SI&cTP=on#ref-10) | DRB |

Vapor pressure @ 20-25 degC (mmHG) 8.13e-006 = **0.001084** Pa [A35] **SOLID**

vapor pressure of 9.22X10-6 mm Hg at 25 deg C = **0.001229** Pa [A5] **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 59 | 107.8 | A3 | 100.1 | 99.2 | 102.0 | 0.73 | A8,A9,A13 | 0.00115 | 0.001084 | 0.001229 | 0.06 | A5,35 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**60 Pyrene**

**Rigid** [A1]  **** Ko=4

Melting Temperature(C) **151.2** [A3]

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **91.2** ± 0.6 [A8], **at 30oC**  SOLID

[A9] Hsub (298K) (Range: 342-418 => 298K –WHY?), kJ/mol **104.5±1.0** **SOLID**

[A9] Hsub (298K), kJ/mol **98.5±1.0** [2003ROJ/ORO] **SOLID**

**Data compiled as indicated in comments:** *[AC](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=AC)* - W.E. Acree, Jr., J.S. Chickos

[*DRB*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=DRB) - D.R. Burgess

[*ALS*](http://webbook.nist.gov/cgi/cbook.cgi?Contrib=ALS) - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Quantity** | **Value** | **Units** | **Method** | **Reference** | **SOLID [A13]; Comment** |
| [A13]: ΔsubH° | **104.5** | kJ/mol | [ME](http://webbook.nist.gov/chemistry/enthalpy.html#ME) | [Siddiqi, Siddiqui, et al., 2009](http://webbook.nist.gov/cgi/cbook.cgi?Name=Pyrene&Units=SI&cTP=on#ref-4) | AC |
| [A13]: ΔsubH° | **100.3 ± 1.0** | kJ/mol | [Review](http://webbook.nist.gov/chemistry/enthalpy.html#Review) | [Roux, Temprado, et al., 2008](http://webbook.nist.gov/cgi/cbook.cgi?Name=Pyrene&Units=SI&cTP=on#ref-5) | There are sufficient high-quality literature values to make a good evaluation with a high degree of confidence. In general, the evaluated uncertainty limits are on the order of (0.5 to 2.5) kJ/mol.; *DRB* |
| [A13]: ΔsubH° | **98.5 ± 1.0** | kJ/mol | [DSC](http://webbook.nist.gov/chemistry/enthalpy.html#DSC) | [Rojas and Orozco, 2003](http://webbook.nist.gov/cgi/cbook.cgi?Name=Pyrene&Units=SI&cTP=on#ref-6) | AC |
| [A13]: ΔsubH° | **100.2 ± 0.4** | kJ/mol | [V](http://webbook.nist.gov/chemistry/enthalpy.html#V) | [Smith, Stewart, et al., 1980](http://webbook.nist.gov/cgi/cbook.cgi?Name=Pyrene&Units=SI&cTP=on#ref-7) | ALS |
| [A13]: ΔsubH° | **100.2** | kJ/mol | N/A | [Smith, Stewart, et al., 1980](http://webbook.nist.gov/cgi/cbook.cgi?Name=Pyrene&Units=SI&cTP=on#ref-7) | DRB |

vapor pressure of 4.5X10-6 mm Hg at 25 deg C = **0.0006 Pa** [A5, A14, A42], **SOLID**

**ΔHvap[25C]: no data Pvap/liq[25C]: no data for LIQUID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 60 | 151.2 | A3 | 101.0 | 98.5 | 104.5 | 1.30 | A8,A9,A13 | 0.0006 | - | - | - | A5,A14,A42 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

**61 Ice/Water**

**Rigid** [A1]  **** Ko=2

Melting Temperature(C) **0 [A24]**

**[A2]:** ΔHsubl[25C] ≡ -ΔHcryst[25C] **51.25** from extrapolation of the P-T dependence for ice (<0oC) [A43] **SOLID**

Melting Enthalpy(kJ/mol) 6.01 [A3]

**25C ΔHvapH (kJ/mol)** **43.98** [A6] *LIQUID*

**Pvap[25C]: 23.8 mm Hg = 3169 Pa** [A44] *LIQUID*

R=8.313472 J/mol.K; =2.47866 kJ/mol (T25=298.15)

 = 0.222

 = **4.0×103 Pa** at 25 oC **SOLID**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 61 | 0 | A24 | 51.2 | - | - | - | A12 | 4000 | - | - | - | A6,A44 |

**DATA on SOLUBILITY and HENRY’S LAW CONSTANTS see in the SUMMARY TABLES in the END**

SUMMARY TABLE for SUBLIMATION – key to colors

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. **Here: comments** | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
|  | in oC |  | in kJ/mol | in kJ/mol | in kJ/mol | dim.less | white: Tmelt>25oC;  H, P for solid | in Pa | in Pa | in Pa | dim. less |  |
|  | in oC |  | in kJ/mol | in kJ/mol | in kJ/mol | dim.less | Light-yellow:  ‑10 oC<Tmelt<25oC  H, P for solid (extrapolated) | in Pa | in Pa | in Pa | dim. less |  |
|  | in oC |  | in kJ/mol | in kJ/mol | in kJ/mol | dim.less | Tmelt<‑10oC | in Pa | in Pa | in Pa | dim. less |  |
| Dark-yellow: H for solid (extrap) |
| Gray: P for liquid only |
|  | in oC |  | in kJ/mol | in kJ/mol | in kJ/mol | dim.less | Green: big error, δln+δΔH/RT>2.5  H, P for solid | in Pa | in Pa | in Pa | dim.less |  |

**SUMMARY TABLE for SUBLIMATION**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | Tmelt | Ref. | <ΔH> | ΔHmin | ΔHmax | ±δΔH/RT | Refs. | <P>geom | Pmin | Pmax | ±δln(P) | Refs. |
| 1 | -93.4 | A3 | 36.695 | - | - | 0.08 | A2 | 353245 | - | - | - | A5 |
| 2 | -114.1 | A3 | 53.807 | - | - | 1.4 | A2 | 7905 | - | - | - | A5 |
| 3 | -98.24 | A4 | 39.567 | - | - | 0.7 | A2 | 66917 | - | - | - | A5 |
| 4 | -84.67 | A4 | 54.024 | - | - | 2 | A2 | 3826 | - | - | - | A5 |
| 5 | -124 | A3 | 26.26 | - | - | 0.04 | A2 | 721153 | - | - | - | A5 |
| 6 | -94.8 | A3 | 39.85 | - | - | 0.19 | A2 | 30792 | - | - | - | A5 |
| 7 | 60.29 | A4 | 56.0 | 55.6 | 56.568 | 1.1 | A8,A9,A10,A13 | 1731.5 | 1730 | 1733 | 0.001 | A11,A12 |
| 8 | -117.1 | A3 | 34.628 | - | - | 0.74 | A2 | 214613 | - | - | - | A5 |
| 9 | 119 | A3 | 80.7 | 80.7 | 80.7 | 0.64 | A8,A9,A13 | 1.39 | 0.200 | 4.022 | 1.37 | A2,A5,A14 |
| 10 | -23.4 | A3 | 55.38 | - | - | 0.45 | A2 | 1113 | - | - | - | A14 |
| 11 | 54.35 | A3 | 75.2 | 74.6 | 75.8 | 0.36 | A8,A9,A13,A15 | 147 | 79.59 | 210 | 0.44 | A2,A7A13,A15 |
| 12 | -108.3 | A3 | 48.807 | - | - | 1.9 | A2 | 21608 | 21594 | 21623 | 0.0001 | A5,A7,A13 |
| 13 | 11.85 | A4 | 49.495 | 49.0 | 49.92 | 0.18 | A2 | 6457 | - | - | - | A4,A7 |
| 14 | -138.2 | A3 | 31.779 | - | - | 0.50 | A2 | 241551 | 240500 | 242606 | 0.005 | A2,A5,A7 |
| 15 | -116.3 | A3 | 41.003 | - | - | 0.04 | A2 | 71578 | 71422 | 71715 | 0.002 | A2,A5 |
| 16 | -41.66 | A3 | 52.434 | - | - | 0.68 | A2 | 2273 | - | - | 0.0002 | A2,A5,A7 |
| 17 | -129.7 | A3 | 39.974 | - | - | 0.11 | A2 | 68353 | - | - | 0.004 | A2,A5,A7 |
| 18 | 115.7 | A3 | 65.2 | 62.760 | 68.645 | 1.0 | A2,A7,A9,A13 | 16.1 | 13.3 | 19.576 | 0.44 | A2,A5,A7 |
| 19 | 5.7 | A3 | 69.49 | 69.27 | 69.71 | 0.09 | A2 | 44.98 | - | - | - | A3,A5,A7 |
| 20 | 44.8 | A3 | 72.8 | 72.3 | 73.3 | 0.25 | A9,A13 | 14.17 | 13.33 | 15.063 | 0.06 | A5,A14 |
| 21 | 5.53 | A3 | 44.6 | 44.4 | 44.8 | 0.04 | A9 | 16720 | - | - | - | A3,A5,A7 |
| 22 | 40.9 | A3 | 68.9 | 68.6 | 69.7 | 0.25 | A9,A13 | 45.77 | 44.7 | 46.83 | 0.02 | A5,A7,A16 |
| 23 | 172.3 | A3 | 97.06 | 94.1 | 103.76 | 1.6 | A9,A13 | 0.00818 | 0.0024 | 0.089 | 1.69 | A5,A14,A17,A18 |
| 24 | 71.2 | A3 | 89.0 | 88.3 | 89.7 | 0.28 | A9,A13 | 0.21 | 0.12 | 0.36 | 0.55 | A5,A19 |
| 25 | 114 | A3 | 96.75 | 96 | 98 | 0.31 | A9,A13 | 0.017 | 0.0031 | 0.123 | 1.52 | A5,A19,A20 |
| 26 | 146 | A3 | 101 | 100 | 102 | 0.4 | A9,A13 | 0.015 | 0.000427 | 0.43 | 2.83 | A5,A22,A23 |
| 27 | -6.02 | A3 | 65.245 | 64.47 | 66.02 | 0.31 | A2 | 147 | - | - | - | A5 |
| 28 | 69.2 | A24 | 88.53 | 87.3 | 89.76 | 0.50 | A9,A13 | 0.25 | - | - | - | A5,A16.A25 |
| 29 | 6.6 | A3 | 37.336 | 36.9 | 37.772 | 0.17 | A2 | 13902 | 13854 | 13952 | 0.004 | A3,A5,A45 |
| 30 | -95.3 | A3 | 48.571 | 48.295 | 48.847 | 0.04 | A2 | 20128 | 19861 | 20395 | 0,013 | A5,A7 |
| 31 | 171 | A24 | 99.1 | 94.3 | 102.2 | 1.84 | A8,A9,A13 | 0.0101 | - | - | - | A5,A14 |
| 32 | 148 | A24 | 91.6 | 87.7 | 97.1 | 1.22 | A8,A9,A13 | 0.55 | 0.197 | 1.54 | 0.6 | A26,A27 |
| 33 | 51.6 | A3 | 78 | 74.8 | 79.1 | 1.09 | A8,A9,A13 | 5.2 | 2.09 | 21.86 | 1.09 | A5,A20,A28 |
| 34 | -95 | A3 | 43.1 | - | - | - | A8,A9,A13 | 3786 | - | - | - | A5,A29 |
| 35 | 29.8 | A3 | 75.4 | 73.7 | 76.02 | 0.39 | A9,A13 | 39.95 | 39.9 | 40.0 | 0.001 | A5,A13,A30 |
| 36 | 35.5 | A3 | 73.7 | 73.1 | 73.9 | 0.36 | A9,A13 | 14.6 | - | - | - | A5,A30 |
| 37 | -90.6 | A3 | 54.125 | - | - | 0.418 | A2,A7 | 6135 | - | - | - | A5 |
| 38 | 20.5 | A32 | 71.076 | - | - | 0.87 | A2 | 61.0 | 57.9 | 64.2 | 0.05 | A3,A5,A32 |
| 39 | 13.25 | A4 | 59.936 | - | - | 0.072 | A2 | 1565 | - | - | - | A4,A5,A10 |
| 40 | 72.8 | A3 | 84.0 | 84.0 | 84.0 | 0.28 | A2,A8,A9,A13 | 6.42 | 3.49 | 11.86 | 0.61 | A4,A10 |
| 41 | 74.8 | A3 | 84.8 | 84.6 | 85.0 | 0.11 | A9,A13 | 9.02 | 3.929 | 20.8 | 0.83 | A7,A5,A14 |
| 42 | 45.7 | A3 | 75.44 | 75.1 | 75.6 | 0.10 | A6,A9,A13 | 29.4 | 23.624 | 36.5 | 0.22 | A2,A7,A5,A14 |
| 43 | 60.8 | A3 | 85.4 | 85.0 | 85.8 | 0.14 | A9,A13 | 2.96 | 1.8358 | 4.78 | 0.48 | A2,A5,A7,A14 |
| 44 | -56.8 | A3 | 66.366 | - | - | 0.05 | A2 | 1880 | - | - | - | A5 |
| 45 | 26.47 | A3 | 77.12 | 73.84 | 80.397 | 1.3 | A2,A3,A6,A7,A9,A33 | 7.49 | 6.06 | 9.25 | 0.21 | A2,A7,A33 |
| 46 | -53.5 | A3 | 68.5 | 65.638 | 71.4 | 0.8 | A2,A8 | 583 | 573.6 | 593 | 0.02 | A5,A7 |
| 47 | 80.2 | A3 | 72.0 | 70.4 | 73.0 | 0.8 | A8,A9,A13 | 11.1 | 10.9 | 11.3 | 0.02 | A5,A7,A14 |
| 48 | -29.7 | A3 | 83.1 | 82.4 | 88.887 | 0.31 | A2,A8 | 186 | 180.91 | 191 | 0.03 | A5,A7 |
| 49 | 83 | A24 | 81.0 | 76.5 | 84.4 | 1.2 | A9,A13 | 0.88 | 0.33 | 2.33 | 0.98 | A5,A34 |
| 50 | 98.5 | A24 | 91.5 | 85.1 | 97.5 | 1.8 | A9,A13 | 0.0086 | 0.00273 | 0.0273 | 0.97 | A14,A35,A36 |
| 51 | 246.2 | A3 | 101.0 | 97.7 | 103.2 | 1.07 | A8,A9,A13 | 0.00255 | 0.000183 | 0.0355 | 2.63 | A5,A14,A35 |
| 52 | 185 | A24 | 112.95 | 111.45 | 114.45 | 0.60 | A9,A13 | 0.00041 | 0.00012 | 0.00140 | 1.07 | A13,A47 |
| 53 | 93.4 | A3 | 85. | 83.4 | 86.0 | 0.49 | A8,A9,A13 | 0.316 | 0.3 | 0.3333 | 0.05 | A5,A38 |
| 54 | 69 | A3 | 81.3 | 77.9 | 82.9 | 0.81 | A8,A9,A13 | 1.26 | 1.19 | 1.333 | 0.06 | A5,A39 |
| 55 | 114.8 | A3 | 84.6 | 80.2 | 87.6 | 1.3 | A8,A9,A13 | 0.136 | 0.043 | 0.432 | 1.1 | A5,A35,A40 |
| 56 | 215 | A3 | 97.9 | 84 | 104.5 | 2.9 | A8,A9,A13 | 0.0083 | 0.00087 | 0.08 | 2.26 | A5,A21 |
| 57 | 99.24 | A3 | 90.3 | 86.6 | 92.5 | 0.98 | A8,A9,A13 | 0.038 | 0,0161 | 0.091 | 0.87 | A5,A35 |
| 58 | 123 | A3 | 100.5 | 98 | 102 | 1.9 | A8,A9,A13 | 0.1173 | - | - | - | A5,A41 |
| 59 | 107.8 | A3 | 100.1 | 99.2 | 102.0 | 0.73 | A8,A9,A13 | 0.00115 | 0.001084 | 0.001229 | 0.06 | A5,35 |
| 60 | 151.2 | A3 | 101.0 | 98.5 | 104.5 | 1.30 | A8,A9,A13 | 0.0006 | - | - | - | A5,A14,A42 |
| 61 | 0 | A24 | 51.2 | - | - | - | A12 | 4000 | - | - | - | A6,A44 |

**BORDER of uncertainty: |δΔH/RT| + |δln(P)| > 2.5**

**SUMMARY TABLE for SOLUBILITY**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No | S, g/L | C (mol/L) | log(C) | Refs. | S, g/L | C (mol/L) | log(C) | Refs. | <log[C]> | ±(log[C]) |
| 1 | 1080,00 | 34,774 | 1,54 | [B1]; strong diss. |  |  |  |  | 1,54 | 0 |
| 2 | 1000,00 | 21,707 | 1,34 | [A5],[B1] |  |  |  |  | 1,34 | 0 |
| 3 | 22,00 | 0,354 | -0,45 | [A5],[B1] |  |  |  |  | -0,45 | 0 |
| 4 | 3,00 | 0,032 | -1,50 | [B1] |  |  |  |  | -1,50 | 0 |
| 5 | 0,38 | 0,009 | -2,04 | [A5],[B1] |  |  |  |  | -2,04 | 0 |
| 6 | 1000,00 | 17,218 | 1,24 | [B1] |  |  |  |  | 1,24 | 0 |
| 7 | 212,00 | 2,350 | 0,37 | [A5] | 175,00 | 1,926 | 0,28 | [B1] | 0,33 | 0.05 |
| 8 | 890,00 | 15,056 | 1,18 | [B1]; strong diss. |  |  |  |  | 1,18 | 0 |
| 9 | 23,80 | 0,238 | -0,62 | [A5],[B1] |  |  |  |  | -0,62 | 0 |
| 10 | 45,00 | 0,671 | -0,17 | [A5],[B1] |  |  |  |  | -0,17 | 0 |
| 11 | 60,30 | 0,511 | -0,29 | [B1] |  |  |  |  | -0,29 | 0 |
| 12 | 1000,00 | 13,868 | 1,14 | [B1] |  |  |  |  | 1,14 | 0 |
| 13 | 1000,00 | 11,350 | 1,05 | [B1] |  |  |  |  | 1,05 | 0 |
| 14 | 0,061 | 0,00105 | -2,98 | [A5],[B1] |  |  |  |  | -2,98 | 0 |
| 15 | 60,40 | 0,815 | -0,09 | [A5],[B1] |  |  |  |  | -0,09 | 0 |
| 16 | 1000,00 | 12,642 | 1,10 | [B1] |  |  |  |  | 1,10 | 0 |
| 17 | 0,038 | 0,00053 | -3,28 | [A5],[B1] |  |  |  |  | -3,28 | 0 |
| 18 | 11,10 | 0,10269 | -0,99 | [A5],[B1] |  |  |  |  | -0,99 | 0 |
| 19 | 2,09 | 0,01698 | -1,77 | [A5],[B1] |  |  |  |  | -1,77 | 0 |
| 20 | 2,50 | 0,01797 | -1,75 | [A5],[B1]; ~50% diss |  |  |  |  | -1,75 | 0 |
| 21 | 1,79 | 0,02292 | -1,64 | [A5],[B1] |  |  |  |  | -1,64 | 0 |
| 22 | 82,80 | 0,87980 | -0,06 | [A5],[B1] |  |  |  |  | -0,06 | 0 |
| 23 | 72,00 | 0,65388 | -0,18 | [A5],[B1] |  |  |  |  | -0,18 | 0 |
| 24 | 1,26 | 0,00912 | -2,04 | [A5] |  |  |  |  | -2,04 | 0 |
| 25 | 1,20 | 0,00869 | -2,06 | [A5],[B1] |  |  |  |  | -2,06 | 0 |
| 26 | 0,73 | 0,00527 | -2,28 | [A5],[B1] |  |  |  |  | -2,28 | 0 |
| 27 | 36,00 | 0,38656 | -0,41 | [A5],[B1] |  |  |  |  | -0,41 | 0 |
| 28 | 772,00 | 6,82226 | 0,83 | [B1] | **4560** | **-** | **-** | [A5],[B3]:>>kg/L | 0,83 | ??? |
| 29 | 0,055 | 0,00065 | -3,18 | [A5],[B1] |  |  |  |  | -3,18 | 0 |
| 30 | 0,0095 | 0,00011 | -3,96 | [A5],[B1] |  |  |  |  | -3,96 | 0 |
| 31 | 2,01 | 0,01701 | -1,77 | [A5],[B1] |  |  |  |  | -1,77 | 0 |
| 32 | 0,83 | 0,00699 | -2,16 | [B1] |  |  |  |  | -2,16 | 0 |
| 33 | 0,44 | 0,00322 | -2,49 | [A5],[B1] |  |  |  |  | -2,49 | 0 |
| 34 | 0,53 | 0,00571 | -2,24 | [A5],[B1] |  |  |  |  | -2,24 | 0 |
| 35 | 25,90 | 0,23951 | -0,62 | [A5],[B1] |  |  |  |  | -0,62 | 0 |
| 36 | 21,50 | 0,19882 | -0,70 | [B1] |  |  |  |  | -0,70 | 0 |
| 37 | 0,0034 | 0,000034 | -4,47 | [A5],[B1] |  |  |  |  | -4,47 | 0 |
| 38 | 6,13 | 0,05102 | -1,29 | [A5],[B1] |  |  |  |  | -1,29 | 0 |
| 39 | 0,16 | 0,00153 | -2,82 | [A5],[B1] |  |  |  |  | -2,82 | 0 |
| 40 | 4,57 | 0,03741 | -1,43 | [A5],[B1] |  |  |  |  | -1,43 | 0 |
| 41 | 3,54 | 0,02898 | -1,54 | [A5],[B1] |  |  |  |  | -1,54 | 0 |
| 42 | 6,05 | 0,04952 | -1,31 | [A5],[B1] |  |  |  |  | -1,31 | 0 |
| 43 | 4,76 | 0,03896 | -1,41 | [A5],[B1] |  |  |  |  | -1,41 | 0 |
| 44 | 0,00066 | 0,0000058 | -5,24 | [A5],[B1] |  |  |  |  | -5,24 | 0 |
| 45 | 4,52 | 0,03500 | -1,46 | [A5],[B1] |  |  |  |  | -1,46 | 0 |
| 46 | 0,00022 | 0,00000175 | -5,76 | [A5];[B1]:0.22g/L-err. | 0,00012 | 0,00000097 | -6,01 | [B2] | -5,89 | 0.13 |
| 47 | 0,031 | 0,00024 | -3,62 | [A5],[B1] |  |  |  |  | -3,62 | 0 |
| 48 | 0,000052 | 0,00000036 | -6,44 | [A5],[B1] | 0,000020 | 0,000000133 | -6,88 | [B2] | -6,66 | 0.22 |
| 49 | 0,0031 | 0,0000184 | -4,73 | [A5],[B1] |  |  |  |  | -4,73 | 0 |
| 50 | 0,00147 | 0,0000080 | -5,10 | [B1] |  |  |  |  | -5,10 | 0 |
| 51 | 0,00180 | 0,0000108 | -4,97 | [B1] |  |  |  |  | -4,97 | 0 |
| 52 | 0,00159 | 0,0000080 | -5,10 | [B1] |  |  |  |  | -5,10 | 0 |
| 53 | 0,00390 | 0,0000253 | -4,60 | [A5],[B1] |  |  |  |  | -4,60 | 0 |
| 54 | 0,00748 | 0,0000486 | -4,31 | [A5] | 0,00694 | 0,0000449 | -4,35 | [B1] | -4,33 | 0.02 |
| 55 | 0,00169 | 0,0000102 | -4,99 | [B1] |  |  |  |  | -4,99 | 0 |
| 56 | 0,001295 | 0,00000726 | -5,14 | [A5] | 0,0000434 | 0,000000244 | -6,61 | [B1] | -5,88 | 0.73 |
| 57 | 0,001000 | 0,00000561 | -5,25 | [A5] | 0,001150 | 0,00000645 | -5,19 | [B1] | -5,22 | 0.03 |
| 58 | 0,000290 | 0,00000161 | -5,79 | [A5],[B1] |  |  |  |  | -5,79 | 0 |
| 59 | 0,000260 | 0,00000129 | -5,89 | [A5],[B1] |  |  |  |  | -5,89 | 0 |
| 60 | 0,000135 | 0,00000067 | -6,18 | [A5],[B1] |  |  |  |  | -6,18 | 0 |
| 61 | 1000,00 | 55,5084 | 1,74 | [B1] |  |  |  |  | 1,74 | 0 |
| No | S, g/L | C (mol/L) | log(C) | Refs. | S, g/L | C (mol/L) | log(C) | Refs. | <log[C]> | ±(log[C]) |

|  |
| --- |
| **Solubility (S) exceeds 200 g/L** |

|  |
| --- |
| strong.dissociation |
| small dissociation |
| big errors |
| small errors |

**SUMMARY TABLE for HENRY’S LAW CONSTANTS**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **TABLE OF LOGARITHMS OF HENRY'S LAW CONSTANTS: ln(kH,cc) = ln(Caq/Cgas)** | | | | | | | | | |
|  |  | No | **ln(Caq/Cgas)** | | **Ref.** | **ln(Caq/Cgas)** | **Ref.** | **ln(Caq/Cgas)** | **Ref.** | **<ln(Caq/Cgas)>** | **±ln(Caq/Cgas)>** |
|  |  | 1 | **7,70** | | [A5] | **7,70** | [B1] | **7,539** | [A2] | **7,64** | 0,07 |
|  |  | 2 | **8,50** | | [A5] | **8,50** | [B1] | **10,76** | [A2] | **9,25** | 1,07 |
|  |  | 3 | **2,72** | | [A5] | **2,72** | [B1] | **2,484** | [A2] | **2,64** | 0,11 |
|  |  | 4 | **3,01** | | [A5] | **3,01** | [B1] | **3,091** | [A2] | **3,03** | 0,04 |
|  |  | 5 | **-3,47** | | [A5] | **-3,47** | [B1] | **-1,24** | [A2] | **-2,73** | 1,05 |
|  |  | 6 | **6,42** | | [A5] | **6,42** | [B1] | **6,51** | [A2] | **6,45** | 0,04 |
|  |  | 7 |  | |  | **11,73** | [B1] | **7,89** | [A2] | **9,81** | 1,92 |
|  |  | 8 | **5,46** | | [A5] | **5,46** | [B1] | **5,45** | [A2] | **5,46** | 0,00 |
|  |  | 9 | **7,35** | | [A5] | **7,35** | [B1] | **11,72** | [A2] | **8,81** | 2,06 |
|  |  | 10 | **7,21** | | [A5] | **7,21** | [B1] | **7,37** | [A2] | **7,27** | 0,07 |
|  |  | 11 | **9,03** | | [A5] | **9,03** | [B1] | **8,69** | [A2] | **8,91** | 0,16 |
|  |  | 12 | **5,85** | | [A5] | **5,85** | [B1] | **8,37** | [A2] | **6,69** | 1,19 |
|  |  | 13 | **8,54** | | [A5] | **8,54** | [B1] | **10,69** | [A2] | **9,25** | 1,02 |
|  |  | 14 | **-3,66** | | [A5] | **-3,66** | [B1] | **-3,3** | [A2] | **-3,54** | 0,17 |
|  |  | 15 | **2,99** | | [A5] | **2,99** | [B1] | **3,14** | [A2] | **3,04** | 0,07 |
|  |  | 16 | **7,71** | | [A5] | **7,71** | [B1] | **7,79** | [A2] | **7,73** | 0,04 |
|  |  | 17 | **-3,93** | | [A5] | **-3,93** | [B1] | **-3,93** | [A2] | **-3,93** | 0,00 |
|  |  | 18 | **3,93** | | [A5] | **3,93** | [B1] | **9,58** | [A2] | **5,82** | 2,66 |
|  |  | 19 | **6,93** | | [A5] | **6,93** | [B1] | **9,27** | [A2] | **7,71** | 1,10 |
|  |  | 20 | **7,31** | | [A5] | **7,56** | [B1] | **6,99** | [A2] | **7,29** | 0,23 |
|  |  | 21 | **1,48** | | [A5] | **1,48** | [B1] | **1,47** | [A2] | **1,48** | 0,01 |
|  |  | 22 | **11,20** | | [A5] | **11,20** | [B1] | **10,98** | [A2] | **11,13** | 0,11 |
|  |  | 23 | **20,28** | | [A5] | **20,06** | [B1] | **20,11** | [A2] | **20,15** | 0,09 |
|  |  | 24 | **12,94** | | [A5] | **12,94** | [B1] | **8,05** | [A2] | **11,31** | 2,30 |
|  |  | 25 | **14,94** | | [A5] | **14,94** | [B1] | **14,98** | [A2] | **14,96** | 0,02 |
|  |  | 26 | **16,78** | | [A5] | **16,78** | [B1] | **11,04** | [A2] | **14,87** | 2,71 |
|  |  | 27 | **9,40** | | [A5] | **9,40** | [B1] | **9,217** | [A2] | **9,34** | 0,09 |
|  |  | 28 | **19,93** | | [A5]:**Caq>kg/L** | **13,78** | [B1] | **19,9** | [A2] | **17,87** | 2,89 |
|  |  | 29 | **-1,81** | | [A5] | **-1,81** | [B1] | **-1,99** | [A2] | **-1,87** | 0,08 |
|  |  | 30 | **-4,30** | | [A5] | **-4,30** | [B1] | **-4,05** | [A2] | **-4,22** | 0,12 |
|  |  | 31 | **11,11** | | [A5] | **11,11** | [B1] | **15,45** | [A2] | **12,55** | 2,05 |
|  |  | 32 | **11,13** | | [A5] | **11,13** | [B1] | **10,34** | [A2] | **10,86** | 0,37 |
|  |  | 33 | **8,38** | | [A5] | **8,38** | [B1] | **8,27** | [A2] | **8,34** | 0,05 |
|  |  | 34 | **1,30** | | [A5] | **1,30** | [B1] | **1,353** | [A2] | **1,32** | 0,02 |
|  |  | 35 | **9,92** | | [A5] | **9,92** | [B1] | **10,01** | [A2] | **9,95** | 0,04 |
|  |  | 36 | **10,10** | | [A5] | **10,10** | [B1] | **10,23** | [A2] | **10,15** | 0,06 |
|  |  | 37 | **-4,30** | | [A5] | **-4,40** | [B1] | **-4,14** | [A2] | **-4,28** | 0,11 |
|  |  | 38 | **7,76** | | [A5] | **7,76** | [B1] | **10,11** | [A2] | **8,55** | 1,11 |
|  |  | 39 | **1,27** | | [A5] | **1,27** | [B1] | **1,29** | [A2] | **1,27** | 0,01 |
|  |  | 40 | **8,97** | | [A5] | **10,41** | [B1] | **10,227** | [A2] | **9,87** | 0,64 |
|  |  | 41 | **8,14** | | [A5] | **9,99** | [B1] | **9,789** | [A2] | **9,31** | 0,83 |
|  |  | 42 | **8,21** | | [A5] | **8,21** | [B1] | **8,557** | [A2] | **8,33** | 0,16 |
|  |  | 43 | **9,92** | | [A5] | **10,98** | [B1] | **10,872** | [A2] | **10,59** | 0,48 |
|  |  | 44 | **-4,88** | | [A5] | **-4,88** | [B1] | **-4,99** | [A2] | **-4,91** | 0,05 |
|  |  | 45 | **10,48** | | [A5] | **10,48** | [B1] | **9,543** | [A2] | **10,17** | 0,44 |
|  |  | 46 | **-4,93** | | [A5], [B2] |  |  | **-5,4** | [A2] | **-5,17** | 0,23 |
|  |  | 47 | **4,02** | | [A5] | **4,02** | [B1] | **3,95** | [A2] | **4,00** | 0,03 |
|  |  | 48 | **-5,35** | | [A5] | **-5,35** | [B1] | **-5,47** | [A2] | **-5,39** | 0,06 |
|  |  | 49 | **4,74** | | [A5] | **4,74** | [B1] | **4,64** | [A2] | **4,71** | 0,05 |
|  |  | 50 | **6,58** | | [A5] | **6,58** | [B1] | **6,423** | [A2] | **6,53** | 0,08 |
|  |  | 51 | **12,55** | | [A5] | **12,55** | [B1] | **8,977** | [A2] | **11,36** | 1,69 |
|  |  | 52 | **13,68** | | [A5] | **13,68** | [B1] | **11,39** | [A2] | **12,92** | 1,08 |
|  |  | 53 | **5,06** | | [A5] | **4,89** | [B1] | **5,04** | [A2] | **5,00** | 0,08 |
|  |  | 54 | **4,37** | | [A5] | **4,37** | [B1] | **3,95** | [A2] | **4,23** | 0,20 |
|  |  | 55 | **5,50** | | [A5] | **5,54** | [B1] | **5,5** | [A2] | **5,51** | 0,02 |
|  |  | 56 | **6,22** | | [A5] | **6,09** | [B1] | **6,47** | [A2] | **6,26** | 0,16 |
|  |  | 57 | **6,36** | | [A5] | **6,36** | [B1] | **6,36** | [A2] | **6,36** | 0,00 |
|  |  | 58 | **3,52** | | [A5] | **3,52** | [B1] | **5,9** | [A2] | **4,32** | 1,12 |
|  |  | 59 | **7,86** | | [A5] | **7,92** | [B1] | **7,89** | [A2] | **7,89** | 0,03 |
|  |  | 60 | **7,63** | | [A5] | **7,63** | [B1] | **7,67** | [A2] | **7,64** | 0,02 |
|  |  | 61 |  | |  |  |  | **10,68** | [A2] | **10,68** | 0 |
| strong.dissociation | | | |
| small dissociation | | | |
| big errors | | | |
| small errors | | | |

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