# Benzene, 1,2-diiodo-

**Other names:** 1,2-Diiodobenzene
Benzene, o-diiodo-
o-Diiodobenzene
**Inchi:** InChI=1S/C6H4I2/c7-5-3-1-2-4-6(5)8/h1-4H
**InchiKey:** BBOLNFYSRZVALD-UHFFFAOYSA-N
**Formula:** C6H4I2
**SMILES:** Ic1ccccc1I
**Mol. weight [g/mol]:** 329.90
**CAS:** 615-42-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3120.00 ± 2.00 | kJ/mol | NIST Webbook |
| gf | 218.66 | kJ/mol | Joback Method |
| hf | 252.00 ± 5.90 | kJ/mol | NIST Webbook |
| hfl | 187.00 ± 4.20 | kJ/mol | NIST Webbook |
| hfus | 13.76 | kJ/mol | Joback Method |
| hvap | 64.90 ± 4.20 | kJ/mol | NIST Webbook |
| log10ws | -3.77 | | Crippen Method |
| logp | 2.896 | | Crippen Method |
| mcvol | 123.280 | ml/mol | McGowan Method |
| pc | 4316.89 | kPa | Joback Method |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| ripol | 2244.00 | | NIST Webbook |
| ripol | 2244.00 | | NIST Webbook |
| tb | 554.62 | K | Joback Method |
| tc | 852.28 | K | Joback Method |
| tf | 297.00 ± 1.50 | K | NIST Webbook |
| tf | 300.00 ± 1.50 | K | NIST Webbook |
| tf | 296.55 ± 0.50 | K | NIST Webbook |
| vc | 0.440 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 209.25 | J/mol×K | 802.67 | Joback Method |
| cpg | 177.80 | J/mol×K | 554.62 | Joback Method |
| cpg | 185.61 | J/mol×K | 604.23 | Joback Method |
| cpg | 192.55 | J/mol×K | 653.84 | Joback Method |
| cpg | 198.74 | J/mol×K | 703.45 | Joback Method |
| cpg | 204.27 | J/mol×K | 753.06 | Joback Method |
| cpg | 213.79 | J/mol×K | 852.28 | Joback Method |
| cpl | 190.00 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0003330 | Pa×s | 554.62 | Joback Method |
| dvisc | 0.0029814 | Pa×s | 312.44 | Joback Method |
| dvisc | 0.0016788 | Pa×s | 352.80 | Joback Method |
| dvisc | 0.0010637 | Pa×s | 393.17 | Joback Method |
| dvisc | 0.0007337 | Pa×s | 433.53 | Joback Method |
| dvisc | 0.0005391 | Pa×s | 473.89 | Joback Method |
| dvisc | 0.0004158 | Pa×s | 514.26 | Joback Method |
| hfust | 14.08 | kJ/mol | 296.55 | NIST Webbook |
| hfust | 14.01 | kJ/mol | 296.60 | NIST Webbook |
| hfust | 14.01 | kJ/mol | 296.60 | NIST Webbook |
| sfust | 47.50 | J/mol×K | 296.55 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 425.20 | K | 2.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.37879e+01 |
| Coeff. B | -4.43145e+03 |

| | |
|---|---|
| Coeff. C | -9.68720e+01 |
| Temperature range (K), min. | 425.12 |
| Temperature range (K), max. | 619.67 |

# Sources

| | |
|---|---|
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C615429&Units=SI |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |