# Biurea, 1,6-bis(2-chloroethyl)-

**Inchi:** InChI=1S/C6H12Cl2N4O2/c7-1-3-9-5(13)11-12-6(14)10-4-2-8/h1-4H2,(H2,9,11,13)(H2,1
**InchiKey:** NFIHKVBHHCVQIS-UHFFFAOYSA-N
**Formula:** C6H12Cl2N4O2
**SMILES:** O=C(NCCCl)NNC(=O)NCCCl
**Mol. weight [g/mol]:** 243.09
**CAS:** 16813-42-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.50 | kJ/mol | Joback Method |
| hf | -209.93 | kJ/mol | Joback Method |
| hfus | 43.28 | kJ/mol | Joback Method |
| hvap | 76.96 | kJ/mol | Joback Method |
| log10ws | -1.89 | | Crippen Method |
| logp | -0.023 | | Crippen Method |
| mcvol | 162.940 | ml/mol | McGowan Method |
| pc | 3501.28 | kPa | Joback Method |
| tb | 719.96 | K | Joback Method |
| tc | 923.05 | K | Joback Method |
| tf | 527.72 | K | Joback Method |
| vc | 0.622 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 413.86 | J/mol×K | 719.96 | Joback Method |
| cpg | 422.83 | J/mol×K | 753.81 | Joback Method |
| cpg | 431.19 | J/mol×K | 787.66 | Joback Method |
| cpg | 438.95 | J/mol×K | 821.50 | Joback Method |
| cpg | 446.14 | J/mol×K | 855.35 | Joback Method |
| cpg | 452.79 | J/mol×K | 889.20 | Joback Method |
| cpg | 458.91 | J/mol×K | 923.05 | Joback Method |

# Sources

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|---|---|
| **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=C16813426&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |