

Acetanilide, 4'-amino-2',6'-dichloro-

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|----------------------|---|
| Inchi: | InChI=1S/C8H8Cl2N2O/c1-4(13)12-8-6(9)2-5(11)3-7(8)10/h2-3H,11H2,1H3,(H,12,13) |
| InchiKey: | GHLHYKAEJJVFCI-UHFFFAOYSA-N |
| Formula: | C8H8Cl2N2O |
| SMILES: | CC(=O)Nc1c(Cl)cc(N)cc1Cl |
| Mol. weight [g/mol]: | 219.07 |
| CAS: | 83386-07-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 103.06 | kJ/mol | Joback Method |
| hf | -63.13 | kJ/mol | Joback Method |
| hfus | 29.64 | kJ/mol | Joback Method |
| hvap | 70.26 | kJ/mol | Joback Method |
| log10ws | -2.68 | | Crippen Method |
| logp | 2.534 | | Crippen Method |
| mcvol | 145.830 | ml/mol | McGowan Method |
| pc | 3713.49 | kPa | Joback Method |
| tb | 675.49 | K | Joback Method |
| tc | 916.19 | K | Joback Method |
| tf | 489.59 | K | Joback Method |
| vc | 0.543 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 326.54 | J/molxK | 675.49 | Joback Method |
| cpg | 335.77 | J/molxK | 715.61 | Joback Method |
| cpg | 344.31 | J/molxK | 755.72 | Joback Method |
| cpg | 352.19 | J/molxK | 795.84 | Joback Method |
| cpg | 359.42 | J/molxK | 835.96 | Joback Method |
| cpg | 366.03 | J/molxK | 876.07 | Joback Method |
| cpg | 372.05 | J/molxK | 916.19 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C83386076&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| 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 |

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