

2H-1,3-Oxazine, tetrahydro-2-phenyl-

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| Other names: | 1,3-Oxazine, tetrahydro-2-phenyl- |
| Inchi: | InChI=1S/C10H13NO/c1-2-5-9(6-3-1)10-11-7-4-8-12-10/h1-3,5-6,10-11H,4,7-8H2 |
| InchiKey: | TVHBYFZBZQWTFS-UHFFFAOYSA-N |
| Formula: | C10H13NO |
| SMILES: | c1ccc(C2NCCCO2)cc1 |
| Mol. weight [g/mol]: | 163.22 |
| CAS: | 17762-72-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 171.77 | kJ/mol | Joback Method |
| hf | -53.07 | kJ/mol | Joback Method |
| hfus | 25.10 | kJ/mol | Joback Method |
| hvap | 51.83 | kJ/mol | Joback Method |
| log10ws | -2.24 | | Crippen Method |
| logp | 1.695 | | Crippen Method |
| mcvol | 132.990 | ml/mol | McGowan Method |
| pc | 3782.33 | kPa | Joback Method |
| tb | 549.93 | K | Joback Method |
| tc | 802.09 | K | Joback Method |
| tf | 367.86 | K | Joback Method |
| vc | 0.478 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 315.92 | J/molxK | 549.93 | Joback Method |
| cpg | 334.52 | J/molxK | 591.96 | Joback Method |
| cpg | 351.79 | J/molxK | 633.98 | Joback Method |
| cpg | 367.77 | J/molxK | 676.01 | Joback Method |
| cpg | 382.50 | J/molxK | 718.04 | Joback Method |
| cpg | 396.03 | J/molxK | 760.07 | Joback Method |
| cpg | 408.41 | J/molxK | 802.09 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.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=C17762720&Units=SI |

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 |
| h vap: | 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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