

1(2H)-Naphthalenone, 3,4-dihydro-

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|-----------------------------|---|
| Other names: | «alpha»-Tetralone 1-Tetralone 1,2,3,4-Tetrahydronaphthalen-1-one 3,4-Dihydro-1(2H)-naphthalenone 3,4-Dihydro-2H-naphthalen-1-one 3,4-Dihydro-1(2H)-naphthaleneone 1,2,3,4-Tetrahydro-1-naphthalenone 1-Oxotetralin 1-Oxo-1,2,3,4-tetrahydronaphthalene alpha-Tetralone 1,2,3,4-Tetrahydro-1-oxonaphthalene 3,4-Dihydronaphthalen-1(2H)-one NSC 5171 |
| Inchi: | InChI=1S/C10H10O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-2,4,6H,3,5,7H2 |
| InchiKey: | XHLHPRDBBAGVEG-UHFFFAOYSA-N |
| Formula: | C10H10O |
| SMILES: | O=C1CCCc2ccccc21 |
| Mol. weight [g/mol]: | 146.19 |
| CAS: | 529-34-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| chs | -5154.70 | kJ/mol | NIST Webbook |
| gf | 69.87 | kJ/mol | Joback Method |
| hf | -75.39 | kJ/mol | Joback Method |
| hfus | 9.78 | kJ/mol | Joback Method |
| hvap | 65.00 ± 0.30 | kJ/mol | NIST Webbook |
| log10ws | -2.83 | | Crippen Method |
| logp | 2.206 | | Crippen Method |
| mcvol | 118.710 | ml/mol | McGowan Method |
| pc | 3722.56 | kPa | Joback Method |
| rinpola | 1458.00 | | NIST Webbook |
| tb | 531.15 | K | NIST Webbook |
| tc | 792.93 | K | Joback Method |
| tf | 278.80 ± 1.00 | K | NIST Webbook |
| vc | 0.445 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 268.39 | J/mol×K | 543.36 | Joback Method |
| cpg | 283.94 | J/mol×K | 584.96 | Joback Method |
| cpg | 298.44 | J/mol×K | 626.55 | Joback Method |
| cpg | 311.91 | J/mol×K | 668.15 | Joback Method |
| cpg | 324.40 | J/mol×K | 709.74 | Joback Method |
| cpg | 335.96 | J/mol×K | 751.34 | Joback Method |
| cpg | 346.61 | J/mol×K | 792.93 | Joback Method |
| hvapt | 61.50 | kJ/mol | 461.50 | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 388.20 | K | 0.80 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C529340&Units=SI |

Legend

| | |
|-------------|--|
| chs: | Standard solid enthalpy of combustion |
| 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 |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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