

1-Silfinene

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C15H24/c1-11-6-7-12-13(2,3)10-14(4)8-5-9-15(11,12)14/h5,9,11-12H,6-8,10H2 |
| InchiKey: | VHIAMHVUKUKCHP-DHMWGJHJSA-N |
| Formula: | C15H24 |
| SMILES: | CC1CCC2C(C)(C)CC3(C)CC=CC123 |
| Mol. weight [g/mol]: | 204.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 231.54 | kJ/mol | Joback Method |
| hf | -84.03 | kJ/mol | Joback Method |
| hfus | 9.28 | kJ/mol | Joback Method |
| hvap | 45.29 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 4.415 | | Crippen Method |
| mcvol | 185.330 | ml/mol | McGowan Method |
| pc | 2239.76 | kPa | Joback Method |
| rinpol | 1350.00 | | NIST Webbook |
| rinpol | 1337.00 | | NIST Webbook |
| tb | 561.90 | K | Joback Method |
| tc | 795.76 | K | Joback Method |
| tf | 369.57 | K | Joback Method |
| vc | 0.709 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 501.64 | J/molxK | 561.90 | Joback Method |
| cpg | 524.98 | J/molxK | 600.88 | Joback Method |
| cpg | 546.53 | J/molxK | 639.85 | Joback Method |
| cpg | 566.74 | J/molxK | 678.83 | Joback Method |
| cpg | 586.06 | J/molxK | 717.81 | Joback Method |
| cpg | 604.93 | J/molxK | 756.78 | Joback Method |
| cpg | 623.79 | J/molxK | 795.76 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R571890&Units=SI |
| 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 |

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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.cheméo.com/cid/33-899-8/1-Silfinene.pdf>

Generated by Cheméo on 2024-04-28 20:41:21.558335206 +0000 UTC m=+16626130.478912523.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.