

Neo-3-Thujol

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C10H18O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-9,11H,4-5H2,1-3H3/t7-,8+,9+,10+ |
| InchiKey: | DZVXRFMREAADPP-XFWSIPNHSA-N |
| Formula: | C10H18O |
| SMILES: | CC1C(O)CC2(C(C)C)CC12 |
| Mol. weight [g/mol]: | 154.25 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -5.35 | kJ/mol | Joback Method |
| hf | -287.08 | kJ/mol | Joback Method |
| hfus | 14.34 | kJ/mol | Joback Method |
| hvap | 52.20 | kJ/mol | Joback Method |
| log10ws | -2.21 | | Crippen Method |
| logp | 2.049 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 2956.90 | kPa | Joback Method |
| rinpol | 1135.00 | | NIST Webbook |
| tb | 524.32 | K | Joback Method |
| tc | 714.97 | K | Joback Method |
| tf | 299.58 | K | Joback Method |
| vc | 0.518 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 354.41 | J/mol×K | 524.32 | Joback Method |
| cpg | 370.07 | J/mol×K | 556.10 | Joback Method |
| cpg | 384.74 | J/mol×K | 587.87 | Joback Method |
| cpg | 398.54 | J/mol×K | 619.65 | Joback Method |
| cpg | 411.57 | J/mol×K | 651.42 | Joback Method |
| cpg | 423.94 | J/mol×K | 683.20 | Joback Method |
| cpg | 435.75 | J/mol×K | 714.97 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R325063&Units=SI |
| 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 |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | 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.chemeo.com/cid/67-948-6/Neo-3-Thujol.pdf>

Generated by Cheméo on 2024-04-30 00:26:40.24370897 +0000 UTC m=+16726049.164286286.

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