

1-Naphthalenepropanol, «alpha»-ethenyldecahydro-«alpha»,5,5,8a-tetramethylene [1S-[1«alpha»(S),4a«beta»,8a«alpha»]]-

Other names: Labd-1-(20),14-dien-13-ol, (13R)-Mandol

Inchi: InChI=1S/C20H34O/c1-7-19(5,21)14-11-16-15(2)9-10-17-18(3,4)12-8-13-20(16,17)6/h7.1

InchiKey: CECREIRZLPLYDM-OQUMVOOASA-N

Formula: C20H34O

SMILES: C=CC(C)(O)CCC1C(=C)CCC2C(C)(C)CCCC12C

Mol. weight [g/mol]: 290.48

CAS: 596-85-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 171.16 | kJ/mol | Joback Method |
| hf | -296.68 | kJ/mol | Joback Method |
| hfus | 19.21 | kJ/mol | Joback Method |
| hvap | 72.58 | kJ/mol | Joback Method |
| log10ws | -6.10 | | Crippen Method |
| logp | 5.502 | | Crippen Method |
| mcvol | 268.210 | ml/mol | McGowan Method |
| pc | 1499.99 | kPa | Joback Method |
| rinpol | 2057.00 | | NIST Webbook |
| rinpol | 2054.00 | | NIST Webbook |
| rinpol | 2087.00 | | NIST Webbook |
| rinpol | 2055.00 | | NIST Webbook |
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| rinpol | 2046.00 | | NIST Webbook |
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| rinpol | 2050.00 | NIST Webbook |
| rinpol | 2055.00 | NIST Webbook |
| rinpol | 2051.00 | NIST Webbook |
| rinpol | 2026.00 | NIST Webbook |
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| rinpol | 2054.00 | | NIST Webbook |
| tb | 763.49 | K | Joback Method |
| tc | 971.09 | K | Joback Method |
| tf | 451.44 | K | Joback Method |
| vc | 1.004 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 857.58 | J/mol×K | 763.49 | Joback Method |
| cpg | 879.64 | J/mol×K | 798.09 | Joback Method |
| cpg | 901.18 | J/mol×K | 832.69 | Joback Method |
| cpg | 922.44 | J/mol×K | 867.29 | Joback Method |
| cpg | 943.64 | J/mol×K | 901.89 | Joback Method |
| cpg | 965.01 | J/mol×K | 936.49 | Joback Method |
| cpg | 986.78 | J/mol×K | 971.09 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C596850&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| mcvol: | McGowan's characteristic volume |

| | |
|-----------------|----------------------------------|
| pc: | Critical Pressure |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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