

epi-Laurenene

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| Inchi: | InChI=1S/C20H32/c1-14-7-6-10-18(4)12-9-16-17(2,3)13-19(5)11-8-15(14)20(16,18)19/h8 |
| InchiKey: | TYDFDHZTDWVUJF-XZANERMPSA-N |
| Formula: | C20H32 |
| SMILES: | CC1CCCC2(C)CCC3C(C)(C)CC4(C)CC=C1C324 |
| Mol. weight [g/mol]: | 272.47 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 307.17 | kJ/mol | Joback Method |
| hf | -116.82 | kJ/mol | Joback Method |
| hfus | 11.58 | kJ/mol | Joback Method |
| hvap | 56.01 | kJ/mol | Joback Method |
| log10ws | -6.18 | | Crippen Method |
| logp | 5.975 | | Crippen Method |
| mcvol | 244.920 | ml/mol | McGowan Method |
| pc | 1724.59 | kPa | Joback Method |
| rmpol | 1891.00 | | NIST Webbook |
| tb | 692.53 | K | Joback Method |
| tc | 936.67 | K | Joback Method |
| tf | 476.76 | K | Joback Method |
| vc | 0.935 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 762.21 | J/mol×K | 692.53 | Joback Method |
| cpg | 788.76 | J/mol×K | 733.22 | Joback Method |
| cpg | 814.91 | J/mol×K | 773.91 | Joback Method |
| cpg | 841.35 | J/mol×K | 814.60 | Joback Method |
| cpg | 868.72 | J/mol×K | 855.29 | Joback Method |
| cpg | 897.71 | J/mol×K | 895.98 | Joback Method |
| cpg | 928.97 | J/mol×K | 936.67 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R570020&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 |

Legend

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|-----------------|---|
| 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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