

(+)-(5R,6S,10S)-«alpha»-gorgonene

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C15H24/c1-11(2)13-8-6-10-15(4)9-5-7-12(3)14(13)15/h13-14H,1,3,5-10H2,2,4 |
| InchiKey: | HRMKWYBxBKFOIS-GIJJTGMTSA-N |
| Formula: | C15H24 |
| SMILES: | <chem>C=C(C)C1CCCC2(C)CCCC(=C)C12</chem> |
| Mol. weight [g/mol]: | 204.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 267.69 | kJ/mol | Joback Method |
| hf | -37.19 | kJ/mol | Joback Method |
| hfus | 13.50 | kJ/mol | Joback Method |
| hvap | 47.61 | kJ/mol | Joback Method |
| log10ws | -4.87 | | Crippen Method |
| logp | 4.725 | | Crippen Method |
| mcvol | 191.890 | ml/mol | McGowan Method |
| pc | 2029.06 | kPa | Joback Method |
| rinpol | 1488.00 | | NIST Webbook |
| rinpol | 1488.00 | | NIST Webbook |
| tb | 564.45 | K | Joback Method |
| tc | 788.06 | K | Joback Method |
| tf | 298.23 | K | Joback Method |
| vc | 0.721 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 497.99 | J/mol×K | 564.45 | Joback Method |
| cpg | 521.74 | J/mol×K | 601.72 | Joback Method |
| cpg | 543.99 | J/mol×K | 638.99 | Joback Method |
| cpg | 564.88 | J/mol×K | 676.25 | Joback Method |
| cpg | 584.58 | J/mol×K | 713.52 | Joback Method |
| cpg | 603.25 | J/mol×K | 750.79 | Joback Method |
| cpg | 621.03 | J/mol×K | 788.06 | Joback Method |

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=R406409&Units=SI |

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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<https://www.chemeo.com/cid/52-584-6/5R-6S-10S-alpha-gorgonene.pdf>

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