

Caryophylla-4(14),8(15)-dien-5«beta»-ol

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|-----------------------------|---|
| Other names: | Caryophylla-4(14),8(15)-dien-5«beta»-ol (=Caryophylladienol I) |
| Inchi: | InChI=1S/C15H26O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h14,16H,1-2,5-11H2,3- |
| InchiKey: | MRNBNSIHBSPJFJ-AWEZLNQCLSA-N |
| Formula: | C15H26O |
| SMILES: | C=C1CCC(O)C(=C)CCCC(C)(C)CC1 |
| Mol. weight [g/mol]: | 222.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -4.49 | kJ/mol | Joback Method |
| hf | -318.26 | kJ/mol | Joback Method |
| hfus | 12.48 | kJ/mol | Joback Method |
| hvap | 65.81 | kJ/mol | Joback Method |
| log10ws | -4.84 | | Crippen Method |
| logp | 4.230 | | Crippen Method |
| mcvol | 208.620 | ml/mol | McGowan Method |
| pc | 2092.66 | kPa | Joback Method |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1638.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1612.00 | | NIST Webbook |
| rinpol | 1641.00 | | NIST Webbook |
| rinpol | 1623.00 | | NIST Webbook |
| rinpol | 1636.00 | | NIST Webbook |
| rinpol | 1636.00 | | NIST Webbook |
| rinpol | 1624.00 | | NIST Webbook |
| rinpol | 1624.00 | | NIST Webbook |
| rinpol | 1628.00 | | NIST Webbook |
| rinpol | 1641.00 | | NIST Webbook |
| ripol | 2267.00 | | NIST Webbook |
| ripol | 2267.00 | | NIST Webbook |
| ripol | 2316.00 | | NIST Webbook |
| ripol | 2316.00 | | NIST Webbook |
| ripol | 2296.00 | | NIST Webbook |
| tb | 669.57 | K | Joback Method |
| tc | 883.39 | K | Joback Method |
| tf | 356.43 | K | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 595.81 | J/mol×K | 669.57 | Joback Method |
| cpg | 617.00 | J/mol×K | 705.21 | Joback Method |
| cpg | 637.09 | J/mol×K | 740.84 | Joback Method |
| cpg | 656.13 | J/mol×K | 776.48 | Joback Method |
| cpg | 674.20 | J/mol×K | 812.12 | Joback Method |
| cpg | 691.35 | J/mol×K | 847.76 | Joback Method |
| cpg | 707.67 | J/mol×K | 883.39 | Joback Method |

Sources

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=R227335&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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 |
| ripola: | 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/36-839-1/Caryophylla-4-14-8-15-dien-5-beta-ol.pdf>

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