

Lupeol

Other names:

Lup-20(29)-en-3-ol, (3«beta»)-
Lup-20(29)-en-3«beta»-ol
«beta»-Viscol
Clerodol
Fagarasterol
Fagarsterol
Lupenol
Monogynol B
Triterpene lupeol
1H-Cyclopenta[a]chrysene, lup-20(29)-en-3-ol deriv.
3«beta»-Lup-20(29)-en-3-ol
NSC 90487
«beta»-Lupeol

Inchi:

InChI=1S/C30H50O/c1-19(2)20-11-14-27(5)17-18-29(7)21(25(20)27)9-10-23-28(6)15-13

InchiKey:

MQYXUWHLBZFQO-RJBYIQQZSA-N

Formula:

C30H50O

SMILES:

C=C(C)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C12

Mol. weight [g/mol]:

426.72

CAS:

545-47-1

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 301.63 | kJ/mol | Joback Method |
| hf | -417.92 | kJ/mol | Joback Method |
| hfus | 27.96 | kJ/mol | Joback Method |
| hvap | 91.45 | kJ/mol | Joback Method |
| log10ws | -8.67 | | Crippen Method |
| logp | 8.025 | | Crippen Method |
| mcvol | 380.830 | ml/mol | McGowan Method |
| pc | 1019.43 | kPa | Joback Method |
| rinpol | 3270.00 | | NIST Webbook |
| rinpol | 3270.00 | | NIST Webbook |
| tb | 1007.04 | K | Joback Method |
| tc | 1245.95 | K | Joback Method |
| tf | 635.60 | K | Joback Method |
| vc | 1.438 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1551.91 | J/mol×K | 1007.04 | Joback Method |
| cpg | 1605.28 | J/mol×K | 1046.86 | Joback Method |
| cpg | 1663.42 | J/mol×K | 1086.68 | Joback Method |
| cpg | 1727.09 | J/mol×K | 1126.50 | Joback Method |
| cpg | 1797.05 | J/mol×K | 1166.31 | Joback Method |
| cpg | 1874.08 | J/mol×K | 1206.13 | Joback Method |
| cpg | 1958.92 | J/mol×K | 1245.95 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C545471&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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |

vc: Critical Volume

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