

2,(7Z,10Z)-Bisabolatrien-13-ol

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C15H24O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5-7,15-16H,4,8-11H2 |
| InchiKey: | QSWUGBKERSBPDI-MLPAPPSSSA-N |
| Formula: | C15H24O |
| SMILES: | CC(C)=CCC=C(C)C1CC=C(CO)CC1 |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 126.72 | kJ/mol | Joback Method |
| hf | -189.67 | kJ/mol | Joback Method |
| hfus | 29.15 | kJ/mol | Joback Method |
| hvap | 67.12 | kJ/mol | Joback Method |
| log10ws | -4.58 | | Crippen Method |
| logp | 4.008 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 2018.13 | kPa | Joback Method |
| rinsol | 1806.00 | | NIST Webbook |
| tb | 666.55 | K | Joback Method |
| tc | 864.71 | K | Joback Method |
| tf | 302.21 | K | Joback Method |
| vc | 0.775 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 565.04 | J/mol×K | 666.55 | Joback Method |
| cpg | 582.17 | J/mol×K | 699.58 | Joback Method |
| cpg | 598.34 | J/mol×K | 732.60 | Joback Method |
| cpg | 613.60 | J/mol×K | 765.63 | Joback Method |
| cpg | 628.02 | J/mol×K | 798.65 | Joback Method |
| cpg | 641.64 | J/mol×K | 831.68 | Joback Method |
| cpg | 654.53 | J/mol×K | 864.71 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R407259&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| hvac: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccol: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/79-130-0/2-7Z-10Z-Bisabolatrien-13-ol.pdf>

Generated by Cheméo on 2024-04-28 01:57:39.742282556 +0000 UTC m=+16558708.662859866.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.