

Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1«alpha»,2«beta»,5«alpha»)-

Other names: 5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol-, (1«alpha»,2«beta»,5«alpha»)-
(1R,2S,5S)-5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol

cis-Sabinene hydrate (cis for IP vs Me)

cis-Sabinene hydrate

Sabinene hydrate, cis

cis-Sabinenhydrate

(1«alpha»,2«beta»,5«alpha»)-2-Methyl-5-(1-methylethyl)bicyclo(3.1.0)hexan-2-ol

Sabinene hydrate trans (trans for IP vs. OH)

trans-Sabinene hydrate (trans for IP vs. OH)

cis-Thujane-4-ol

cis-4-Thujanol

15537-55-0

Sabinene hydrate trans

Inchi: InChI=1S/C10H18O/c1-7(2)10-5-4-9(3,11)8(10)6-10/h7-8,11H,4-6H2,1-3H3/t8?,9-,10-/m

InchiKey: KXSDPILWGMGFJMM-VXRWAFEHSA-N

Formula: C10H18O

SMILES: CC(C)C12CCC(C)(O)C1C2

Mol. weight [g/mol]: 154.25

CAS: 15537-55-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -3.13 | kJ/mol | Joback Method |
| hf | -251.50 | kJ/mol | Joback Method |
| hfus | 6.97 | kJ/mol | Joback Method |
| hvap | 51.36 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.194 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 3224.64 | kPa | Joback Method |
| rinpol | 1054.00 | | NIST Webbook |
| rinpol | 1066.00 | | NIST Webbook |
| rinpol | 1070.30 | | NIST Webbook |
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| ripol | 1426.00 | | NIST Webbook |
| ripol | 1423.00 | | NIST Webbook |
| ripol | 1469.00 | | NIST Webbook |
| tb | 529.23 | K | Joback Method |
| tc | 727.62 | K | Joback Method |
| tf | 327.72 | K | Joback Method |
| vc | 0.517 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

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|-----|--------|---------|--------|---------------|
| cpg | 353.14 | J/mol×K | 529.23 | Joback Method |
| cpg | 368.19 | J/mol×K | 562.29 | Joback Method |
| cpg | 382.12 | J/mol×K | 595.36 | Joback Method |
| cpg | 395.11 | J/mol×K | 628.42 | Joback Method |
| cpg | 407.37 | J/mol×K | 661.49 | Joback Method |
| cpg | 419.07 | J/mol×K | 694.55 | Joback Method |
| cpg | 430.42 | J/mol×K | 727.62 | 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=C15537550&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307i |

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 |
| ripol: | 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/70-635-9/Bicyclo-3-1-0-hexan-2-ol-2-methyl-5-1-methylethyl-1-alpha-2-beta-5-alpha.pdf>

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