

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

Other names: (1R,2R,5S)-5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol
trans-Sabinene hydrate (trans for Me vs IP)

trans-Sabinene hydrate

trans-Sabinene hydroxide

Sabinene hydrate, trans

5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol, (1«alpha»,2«alpha»,5«alpha»)-

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

trans-4-Thujanol

cis-Sabinene hydrate (cis for OH vs IP)

cis-Sabinene hydrate

trans-Sabinenhydrate

Sabinene hydrate-cis

cis-Sabinene hydroxide

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

InchiKey: KXSDPILWGMGFJMM-UHFFFAOYSA-N

Formula: C10H18O

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

Mol. weight [g/mol]: 154.25

CAS: 17699-16-0

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
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tf	327.72	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

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=C17699160&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
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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