

Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1«alpha»,3«alpha»,5«alpha»)-

Other names: (1R,3R,5R)-1-Isopropyl-4-methylenebicyclo[3.1.0]hexan-3-ol
4(10)-Thujen-3-ol, stereoisomer

(-)-cis-Sabinol

1-Isopropyl-4-methylenebicyclo[3.1.0]hexan-3-ol-, (1«alpha»,3«alpha»,5«alpha»)-
cis-Sabinol

Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1R,3R,5R)-rel(-)-
4(10)-Thujen-3-ol

Inchi:	InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6,8-9,11H,3-5H2,1-2H3/t8-,9+,10+
InchiKey:	MDFQXBNOAKNAY-IVZWLZJFSA-N
Formula:	C10H16O
SMILES:	C=C1C(O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	152.23
CAS:	3310-02-9

Physical Properties

Property code	Value	Unit	Source
gf	55.44	kJ/mol	Joback Method
hf	-182.50	kJ/mol	Joback Method
hfus	12.11	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mvol	131.610	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1128.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1179.00		NIST Webbook

ripol	1137.00		NIST Webbook
ripol	1143.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	528.15	K	Joback Method
tc	720.59	K	Joback Method
tf	317.50	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.82	J/mol×K	528.15	Joback Method
cpg	348.84	J/mol×K	560.22	Joback Method
cpg	361.94	J/mol×K	592.30	Joback Method
cpg	374.24	J/mol×K	624.37	Joback Method
cpg	385.85	J/mol×K	656.45	Joback Method
cpg	396.88	J/mol×K	688.52	Joback Method
cpg	407.43	J/mol×K	720.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3310029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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