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

Other names:	4(10)-Thujen-3-ol, (1S,3R,5S)-(+)- (+)-Sabinol trans-Sabinol Sabinol Sabinol, (+)- thuj-4(10)-en-3-ol (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
InchiKey:	MDFQXBNVOAKNAY-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=C1C(O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	152.23
CAS:	471-16-9

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
mcvol	131.610	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1136.00		NIST Webbook

rinpol	1134.00		NIST Webbook
rinpol	1143.10		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1114.00		NIST Webbook
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rinpol	1170.00		NIST Webbook
rinpol	1142.00		NIST Webbook
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rinpol	1178.00		NIST Webbook
rinpol	1143.00		NIST Webbook
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rinpol	1143.00		NIST Webbook
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rinpol	1143.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1790.00		NIST Webbook
tb	528.15	K	Joback Method
tc	720.59	K	Joback Method
tf	317.50	K	Joback Method
vc	0.503	m3/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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3310029&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

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

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