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

Other names: 4-Thujanol
Sabinene hydrate
(Z)-Sabinene hydrate
2-methyl-5-(1-methylethyl)bicyclo[3.1.0]hexan-2-ol

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: KXSDPILWMGFJMM-UHFFFAOYSA-N

Formula: C10H18O

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

Mol. weight [g/mol]: 154.25

CAS: 546-79-2

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	1053.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1077.00		NIST Webbook

rinpol	1082.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1125.00		NIST Webbook
ripol	1469.00		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	m3/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=C546792&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
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