Bicyclo[3.1.1]heptane-2-methanol, 6,6-dimethyl-, [1S-(1«alpha»,2«alpha»,5«alpha»)]-

Other names:	(1S,2S,5S)-(-)-Myrtanol (-)-trans-Myrtanol (6,6-Dimethylbicyclo[3.1.1]hept-2-yl)methanol, [1S-(1«alpha»,2«alpha»,5«alpha»)]- [1S-(1«alpha»,2«alpha»,5«alpha»)]-6,6-dimethylbicyclo[3.1.1]heptane-2-methanol trans-Myrtanol
Inchi:	InChI=1S/C10H18O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h7-9,11H,3-6H2,1-2H3/t7-,8+,9+/m1/s
InchiKey:	LDWAIHWGMRVEFR-VGMNWLOBSA-N
Formula:	C10H18O
SMILES:	CC1(C)C2CCC(CO)C1C2
Mol. weight [g/mol]:	154.25
CAS:	53369-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-15.01	kJ/mol	Joback Method
hf	-287.96	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	52.76	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.051		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1239.00		NIST Webbook

rinpol	1258.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1868.00		NIST Webbook
tb	529.03	K	Joback Method
tc	722.31	K	Joback Method
tf	311.06	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.68	J/mol×K	529.03	Joback Method
cpg	370.78	J/mol×K	561.24	Joback Method
cpg	385.90	J/mol×K	593.46	Joback Method
cpg	400.13	J/mol×K	625.67	Joback Method
cpg	413.58	J/mol×K	657.88	Joback Method
cpg	426.35	J/mol×K	690.10	Joback Method
cpg	438.56	J/mol×K	722.31	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=C53369178&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