

(-)-Myrtenol

Other names:	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-, (1R)-(1R)-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-methanol
Inchi:	InChI=1S/C10H16O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h3,8-9,11H,4-6H2,1-2H3
InchiKey:	RXBQNMWIKOSCS-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1(C)C2CC=C(CO)C1C2
Mol. weight [g/mol]:	152.23
CAS:	19894-97-4

Physical Properties

Property code	Value	Unit	Source
gf	13.03	kJ/mol	Joback Method
hf	-221.31	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	54.02	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.971		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1212.80		NIST Webbook
rinpol	1212.80		NIST Webbook
tb	537.84	K	Joback Method
tc	734.16	K	Joback Method
tf	328.58	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.67	J/molxK	537.84	Joback Method
cpg	349.94	J/molxK	570.56	Joback Method
cpg	363.29	J/molxK	603.28	Joback Method
cpg	375.84	J/molxK	636.00	Joback Method
cpg	387.71	J/molxK	668.72	Joback Method

cpg	399.00	J/mol×K	701.44	Joback Method
cpg	409.83	J/mol×K	734.16	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=C19894974&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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