trans-Myrtanol

Other names:	(-)-trans-Myrtanol (1S,2S,5S)-(-)-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
InchiKey:	LDWAIHWGMRVEFR-VGMNWLOBSA-N
Formula:	C10H18O
SMILES:	CC1(C)C2CCC(CO)C1C2
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
hfus	15.76	kJ/mol	Joback Method
logp	2.051		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
tb	496.11	K	Cheméo Relay (1.0)
tf	387.58	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15358915&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point