

cis-Myrtanyl isobutyrate

Inchi:	InChI=1S/C13H22O2/c1-8(2)12(14)15-11-6-5-9-7-10(11)13(9,3)4/h8-11H,5-7H2,1-4H3/tS
InchiKey:	GUQHUQNPSNWPID-MXWKQRLJSA-N
Formula:	C13H22O2
SMILES:	CC(C)C(=O)OC1CCC2CC1C2(C)C
Mol. weight [g/mol]:	210.31

Physical Properties

Property code	Value	Unit	Source
gf	-89.29	kJ/mol	Joback Method
hf	-447.73	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.010		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinsol	1524.00		NIST Webbook
tb	581.34	K	Joback Method
tc	789.76	K	Joback Method
tf	341.21	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.15	J/molxK	581.34	Joback Method
cpg	509.86	J/molxK	616.08	Joback Method
cpg	528.45	J/molxK	650.81	Joback Method
cpg	546.02	J/molxK	685.55	Joback Method
cpg	562.72	J/molxK	720.29	Joback Method
cpg	578.65	J/molxK	755.03	Joback Method
cpg	593.95	J/molxK	789.76	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587365&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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