Myrtenyl 3-methylvalerate

Inchi: InChI=1S/C16H26O2/c1-5-11(2)8-15(17)18-10-12-6-7-13-9-14(12)16(13,3)4/h6,11,13-14
InchiKey: AMMGLFBUAHGYBC-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCC(C)CC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-35.99	kJ/mol	Joback Method
hf	-443.00	kJ/mol	Joback Method
hfus	26.24	kJ/mol	Joback Method
hvap	59.47	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.958		Crippen Method
mcvol	217.720	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1673.70		NIST Webbook
rinpol	1673.70		NIST Webbook
tb	658.79	K	Joback Method
tc	860.90	K	Joback Method
tf	392.54	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.20	J/mol×K	658.79	Joback Method
cpg	646.32	J/mol×K	692.48	Joback Method
cpg	664.53	J/mol×K	726.16	Joback Method
cpg	681.94	J/mol×K	759.85	Joback Method
cpg	698.68	J/mol×K	793.53	Joback Method
cpg	714.86	J/mol×K	827.22	Joback Method
cpg	730.61	J/mol×K	860.90	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=U414245&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
mcvol:	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