Myrtenyl 2-methyl butyrate

Inchi: InChI=1S/C15H24O2/c1-5-10(2)14(16)17-9-11-6-7-12-8-13(11)15(12,3)4/h6,10,12-13H,5
InchiKey: NMVOOLZURJHGKQ-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CCC(C)C(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 236.35
CAS: 138530-44-6

Physical Properties

Property code	Value	Unit	Source
gf	-44.41	kJ/mol	Joback Method
hf	-422.36	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	57.24	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.568		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1559.50		NIST Webbook
rinpol	1559.50		NIST Webbook
tb	635.91	K	Joback Method
tc	840.83	K	Joback Method
tf	381.27	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/mol×K	635.91	Joback Method
cpg	591.81	J/mol×K	670.06	Joback Method
cpg	609.60	J/mol×K	704.22	Joback Method
cpg	626.56	J/mol×K	738.37	Joback Method
cpg	642.81	J/mol×K	772.52	Joback Method
cpg	658.48	J/mol×K	806.67	Joback Method
cpg	673.69	J/mol×K	840.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C138530446&Units=SI
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

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