myrtenyl 3-methylbutanoate

Inchi: InChI=1S/C15H24O2/c1-10(2)7-14(16)17-9-11-5-6-12-8-13(11)15(12,3)4/h5,10,12-13H,6
InchiKey: TVGPYTOYKLZBPA-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC(C)CC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 236.35
CAS: 33900-84-4

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	1552.10		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1552.10		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1521.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1855.00		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

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=C33900844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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