«beta»-Isocyclolavandulyl isobutyrate

Inchi: InChI=1S/C14H24O2/c1-10(2)13(15)16-9-12-6-7-14(4,5)8-11(12)3/h6,10-11H,7-9H2,1-5H
InchiKey: QTBRAZDTZAOKEV-NSHDSACASA-N
Formula: C14H24O2
SMILES: CC(C)C(=O)OCC1=CCC(C)(C)CC1C
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-137.78	kJ/mol	Joback Method
hf	-486.84	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.568		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
ripol	1691.00		NIST Webbook
ripol	1691.00		NIST Webbook
tb	614.83	K	Joback Method
tc	822.36	K	Joback Method
tf	345.02	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.02	J/mol×K	614.83	Joback Method
cpg	557.47	J/mol×K	649.42	Joback Method
cpg	575.94	J/mol×K	684.01	Joback Method
cpg	593.52	J/mol×K	718.60	Joback Method
cpg	610.30	J/mol×K	753.19	Joback Method
cpg	626.36	J/mol×K	787.78	Joback Method

cpg	641.79	J/mol×K	822.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418878&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume