«beta»-Isocyclolavandulyl propionate

Inchi: InChI=1S/C13H22O2/c1-5-12(14)15-9-11-6-7-13(3,4)8-10(11)2/h6,10H,5,7-9H2,1-4H3/t1
InchiKey: XOZBCNJUNGIXPL-JTQLQIEISA-N
Formula: C13H22O2
SMILES: CCC(=O)OCC1=CCC(C)(C)CC1C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-143.76	kJ/mol	Joback Method
hf	-460.92	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.322		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1694.00		NIST Webbook
tb	592.39	K	Joback Method
tc	799.01	K	Joback Method
tf	348.75	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.49	J/mol×K	592.39	Joback Method
cpg	504.04	J/mol×K	626.83	Joback Method
cpg	521.65	J/mol×K	661.26	Joback Method
cpg	538.40	J/mol×K	695.70	Joback Method
cpg	554.38	J/mol×K	730.14	Joback Method
cpg	569.67	J/mol×K	764.58	Joback Method

cpg	584.35	J/mol×K	799.01	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=R418898&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