«beta»-Cyclolavandulyl isobutyrate

Inchi: InChI=1S/C14H24O2/c1-10(2)13(15)16-9-12-6-7-14(4,5)8-11(12)3/h10H,6-9H2,1-5H3
InchiKey: MPXQTTNSJUOAST-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: CC1=C(COC(=O)C(C)C)CCC(C)(C)C1
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-139.70	kJ/mol	Joback Method
hf	-477.97	kJ/mol	Joback Method
hfus	17.26	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.712		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1702.00		NIST Webbook
tb	624.48	K	Joback Method
tc	833.00	K	Joback Method
tf	361.78	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.65	J/mol×K	624.48	Joback Method
cpg	555.42	J/mol×K	659.23	Joback Method
cpg	573.27	J/mol×K	693.99	Joback Method
cpg	590.29	J/mol×K	728.74	Joback Method
cpg	606.58	J/mol×K	763.50	Joback Method
cpg	622.21	J/mol×K	798.25	Joback Method

cpg	637.28	J/mol×K	833.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418823&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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