Perillyl isobutyrate

Inchi: InChI=1S/C14H22O2/c1-10(2)13-7-5-12(6-8-13)9-16-14(15)11(3)4/h5,11,13H,1,6-9H2,2-
InchiKey: KAQYLYYVKDTFRT-CYBMUJFWSA-N
Formula: C14H22O2
SMILES: C=C(C)C1CC=C(COC(=O)C(C)C)CC1
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-45.29	kJ/mol	Joback Method
hf	-366.10	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.488		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1567.00		NIST Webbook
tb	615.82	K	Joback Method
tc	823.34	K	Joback Method
tf	309.64	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.01	J/mol×K	615.82	Joback Method
cpg	535.92	J/mol×K	650.41	Joback Method
cpg	553.77	J/mol×K	684.99	Joback Method
cpg	570.58	J/mol×K	719.58	Joback Method
cpg	586.38	J/mol×K	754.17	Joback Method
cpg	601.19	J/mol×K	788.75	Joback Method
cpg	615.03	J/mol×K	823.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587409&Units=SI

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