Epoxypseudoisoeugenyl 2-methylbutyrate

Inchi: InChI=1S/C14H18O4/c1-8(2)14(15)18-11-6-5-10(7-12(11)16-4)13-9(3)17-13/h5-9,13H,1-
InchiKey: MCVNHWFLEYXICF-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: COc1cc(C2OC2C)ccc1OC(=O)C(C)C
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-214.29	kJ/mol	Joback Method
hf	-580.54	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.716		Crippen Method
mcvol	192.680	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1844.00		NIST Webbook
ripol	2698.00		NIST Webbook
ripol	2698.00		NIST Webbook
ripol	2698.00		NIST Webbook
tb	683.65	K	Joback Method
tc	898.45	K	Joback Method
tf	418.66	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.12	J/mol×K	683.65	Joback Method
cpg	556.21	J/mol×K	719.45	Joback Method

cpg	571.30	J/mol×K	755.25	Joback Method
cpg	585.42	J/mol×K	791.05	Joback Method
cpg	598.59	J/mol×K	826.85	Joback Method
cpg	610.82	J/mol×K	862.65	Joback Method
cpg	622.14	J/mol×K	898.45	Joback Method
dvisc	0.0013517	Pa×s	418.66	Joback Method
dvisc	0.0009491	Pa×s	462.83	Joback Method
dvisc	0.0007088	Pa×s	506.99	Joback Method
dvisc	0.0005547	Pa×s	551.15	Joback Method
dvisc	0.0004502	Pa×s	595.32	Joback Method
dvisc	0.0003760	Pa×s	639.49	Joback Method
dvisc	0.0003215	Pa×s	683.65	Joback Method

Sources

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=R240041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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