4-Methoxy-2-(3-methyloxiranyl)-phenyl isobutyrate

Inchi: InChI=1S/C14H18O4/c1-8(2)14(15)18-12-6-5-10(16-4)7-11(12)13-9(3)17-13/h5-9,13H,1-

InchiKey: WSPQJFZGVXTTPB-UHFFFAOYSA-N

Formula: C14H18O4

SMILES: COc1ccc(OC(=O)C(C)C)c(C2OC2C)c1

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
ripol	2613.00		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

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=R418318&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume