

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/molxK	683.65	Joback Method
cpg	610.82	J/molxK	862.65	Joback Method
cpg	598.59	J/molxK	826.85	Joback Method
cpg	585.42	J/molxK	791.05	Joback Method
cpg	571.30	J/molxK	755.25	Joback Method
cpg	556.21	J/molxK	719.45	Joback Method
cpg	622.14	J/molxK	898.45	Joback Method
dvisc	0.0003215	Paxs	683.65	Joback Method
dvisc	0.0003760	Paxs	639.49	Joback Method

dvisc	0.0004502	Paxs	595.32	Joback Method
dvisc	0.0005547	Paxs	551.15	Joback Method
dvisc	0.0007088	Paxs	506.99	Joback Method
dvisc	0.0009491	Paxs	462.83	Joback Method
dvisc	0.0013517	Paxs	418.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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