4-(3-Methyloxiranyl)-phenyl-2-methyl butyrate

Inchi: InChI=1S/C14H18O3/c1-4-9(2)14(15)17-12-7-5-11(6-8-12)13-10(3)16-13/h5-10,13H,4H2
InchiKey: GZZHKMKHBABOEJ-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: CCC(C)C(=O)Oc1ccc(C2OC2C)cc1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-99.66	kJ/mol	Joback Method
hf	-436.85	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.098		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
ripol	2506.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2506.00		NIST Webbook
tb	656.25	K	Joback Method
tc	872.63	K	Joback Method
tf	383.91	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.69	J/mol×K	656.25	Joback Method
cpg	530.35	J/mol×K	692.31	Joback Method
cpg	545.97	J/mol×K	728.38	Joback Method
cpg	560.56	J/mol×K	764.44	Joback Method
cpg	574.19	J/mol×K	800.50	Joback Method
cpg	586.89	J/mol×K	836.57	Joback Method
cpg	598.71	J/mol×K	872.63	Joback Method

dvisc	0.0019702	Pa×s	383.91	Joback Method
dvisc	0.0013106	Pa×s	429.30	Joback Method
dvisc	0.0009425	Pa×s	474.69	Joback Method
dvisc	0.0007179	Pa×s	520.08	Joback Method
dvisc	0.0005713	Pa×s	565.47	Joback Method
dvisc	0.0004703	Pa×s	610.86	Joback Method
dvisc	0.0003977	Pa×s	656.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418274&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
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