Octanoic acid, 2,3-epoxy-, methyl ester

Inchi: InChI=1S/C9H16O3/c1-3-4-5-6-7-8(12-7)9(10)11-2/h7-8H,3-6H2,1-2H3
InchiKey: CBKAPKPTOHISFB-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CCCCCC1OC1C(=O)OC
Mol. weight [g/mol]: 172.22
CAS: 116663-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-242.10	kJ/mol	Joback Method
hf	-553.43	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.507		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	510.63	K	Joback Method
tc	696.74	K	Joback Method
tf	303.62	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.15	J/mol×K	510.63	Joback Method
cpg	354.26	J/mol×K	541.65	Joback Method
cpg	367.74	J/mol×K	572.67	Joback Method
cpg	380.59	J/mol×K	603.69	Joback Method
cpg	392.83	J/mol×K	634.71	Joback Method
cpg	404.48	J/mol×K	665.73	Joback Method
cpg	415.55	J/mol×K	696.74	Joback Method
dvisc	0.0019988	Pa×s	303.62	Joback Method
dvisc	0.0014333	Pa×s	338.12	Joback Method

dvisc	0.0010931	Pa×s	372.62	Joback Method
dvisc	0.0008729	Pa×s	407.12	Joback Method
dvisc	0.0007219	Pa×s	441.63	Joback Method
dvisc	0.0006137	Pa×s	476.13	Joback Method
dvisc	0.0005333	Pa×s	510.63	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=C116663037&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume