Methyl (11R,12R,13S)-(Z)-12,13-epoxy-11-methoxy-9-octa

Other names: Methyl (Z)-12,13-epoxy-11-methoxy-9-octadecenoate
Inchi: InChI=1S/C20H36O4/c1-4-5-11-15-18-20(24-18)17(22-2)14-12-9-7-6-8-10-13-16-19(21)2
InchiKey: BOCZHGZTZHPCHP-WYMLVPIESA-N
Formula: C20H36O4
SMILES: CCCCCC1OC1C(C=CCCCCCCCC(=O)OC)OC
Mol. weight [g/mol]: 340.50
CAS: 88335-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-176.70	kJ/mol	Joback Method
hf	-800.75	kJ/mol	Joback Method
hfus	55.39	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.809		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2525.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	788.45	K	Joback Method
tc	973.76	K	Joback Method
tf	429.74	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.48	J/mol×K	788.45	Joback Method
cpg	1027.31	J/mol×K	942.87	Joback Method
cpg	1012.20	J/mol×K	911.99	Joback Method
cpg	996.20	J/mol×K	881.10	Joback Method
cpg	979.28	J/mol×K	850.22	Joback Method

cpg	961.38	J/mol×K	819.33	Joback Method
cpg	1041.57	J/mol×K	973.76	Joback Method
dvisc	0.0001439	Pa×s	788.45	Joback Method
dvisc	0.0001802	Pa×s	728.66	Joback Method
dvisc	0.0002349	Pa×s	668.88	Joback Method
dvisc	0.0003226	Pa×s	609.10	Joback Method
dvisc	0.0004747	Pa×s	549.31	Joback Method
dvisc	0.0007676	Pa×s	489.53	Joback Method
dvisc	0.0014187	Pa×s	429.74	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=C88335391&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume