

Oxiraneoctanoic acid, 3-octyl-, cis-

Other names:	Octadecanoic acid, 9,10-epoxy-, cis- cis-9,10-Epoxyoctadecanoic Acid cis-9,10-Epoxystearic Acid Epoxyoleic acid 8-(3-Octyl-2-oxiranyl)octanoic acid, cis 2-Oxiraneoctanoic acid, 3-octyl-, (2R,3S)-rel-
Inchi:	InChI=1S/C18H34O3/c1-2-3-4-5-7-10-13-16-17(21-16)14-11-8-6-9-12-15-18(19)20/h16-1
InchiKey:	IMZYCNQZDBZBQ-DLBZAZTESA-N
Formula:	C18H34O3
SMILES:	CCCCCCCC1OC1CCCCCCCC(=O)O
Mol. weight [g/mol]:	298.46
CAS:	24560-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-198.14	kJ/mol	Joback Method
hf	-759.20	kJ/mol	Joback Method
hfus	55.25	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.320		Crippen Method
mcvol	266.930	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
tb	786.31	K	Joback Method
tc	966.58	K	Joback Method
tf	443.64	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.12	J/mol×K	786.31	Joback Method
cpg	934.60	J/mol×K	936.53	Joback Method
cpg	920.81	J/mol×K	906.49	Joback Method

cpg	906.31	J/molxK	876.44	Joback Method
cpg	891.06	J/molxK	846.40	Joback Method
cpg	875.01	J/molxK	816.35	Joback Method
cpg	947.71	J/molxK	966.58	Joback Method
dvisc	0.0000750	Paxs	786.31	Joback Method
dvisc	0.0001055	Paxs	729.20	Joback Method
dvisc	0.0001575	Paxs	672.09	Joback Method
dvisc	0.0002531	Paxs	614.97	Joback Method
dvisc	0.0004484	Paxs	557.86	Joback Method
dvisc	0.0009048	Paxs	500.75	Joback Method
dvisc	0.0021878	Paxs	443.64	Joback Method

Sources

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=C24560983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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