Oleyl oleate

Other names:	9-Octadecenoic acid (Z)-, 9-octadecenyl ester, (Z)-
	Oleic acid, (Z)-9-octadecenyl ester
	Cetiol
	Oleic acid oleyl ester
	Schercemol OLO ester
	Wickenol 143
	(9Z)-9-Octadecenyl (9Z)-9-octadecenoate
	(Z)-Octadec-9-enyl oleate
	9-Octadecenoic acid (9Z)-, (9Z)-9-octadecen-1-yl ester
	9-Octadecenoic acid (9Z)-, (9Z)-9-octadecenyl ester
	Octadec-9-enoic acid octadec-9-enyl ester, Z,Z
Inchi:	InChI=1S/C36H68O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-
InchiKey:	BARWIPMJPCRCTP-CLFAGFIQSA-N
Formula:	C36H68O2
SMILES:	CCCCCCCCC=CCCCCCCCCOC(=O)CCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]:	532.92
CAS:	3687-45-4

Physical Properties

Property code	Value	Unit	Source
gf	178.76	kJ/mol	Joback Method
hf	-796.73	kJ/mol	Joback Method
hfus	92.19	kJ/mol	Joback Method
hvap	104.80	kJ/mol	Joback Method
log10ws	-13.46		Crippen Method
logp	12.605		Crippen Method
mcvol	516.940	ml/mol	McGowan Method
pc	488.60	kPa	Joback Method
rinpol	3695.89		NIST Webbook
rinpol	3695.89		NIST Webbook
tb	1107.69	K	Joback Method
tc	1426.10	K	Joback Method
tf	557.48	K	Joback Method
vc	2.035	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1899.39	J/mol×K	1107.69	Joback Method
cpg	2046.86	J/mol×K	1373.03	Joback Method
cpg	2020.40	J/mol×K	1319.96	Joback Method
cpg	1992.82	J/mol×K	1266.90	Joback Method
cpg	1963.73	J/mol×K	1213.83	Joback Method
cpg	1932.72	J/mol×K	1160.76	Joback Method
cpg	2072.61	J/mol×K	1426.10	Joback Method
dvisc	0.0000050	Pa×s	1107.69	Joback Method
dvisc	0.0000069	Pa×s	1015.99	Joback Method
dvisc	0.0000103	Pa×s	924.29	Joback Method
dvisc	0.0000166	Pa×s	832.59	Joback Method
dvisc	0.0000301	Pa×s	740.88	Joback Method
dvisc	0.0000649	Pa×s	649.18	Joback Method
dvisc	0.0001798	Pa×s	557.48	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=C3687454&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