

Eicosanoic acid, 9-octadecenyl ester, (Z)-

Other names:	Oleyl arachidate octadec-9-enyl icosanoate Icosanoic acid octadec-9-enyl ester, Z
Inchi:	InChI=1S/C38H74O2/c1-3-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-36-38(39)40-
InchiKey:	HWRYIWKGLJIMLG-ZZEZOPTASA-N
Formula:	C38H74O2
SMILES:	CCCCCCCCC=CCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	562.99
CAS:	22393-96-0

Physical Properties

Property code	Value	Unit	Source
gf	115.38	kJ/mol	Joback Method
hf	-955.23	kJ/mol	Joback Method
hfus	97.17	kJ/mol	Joback Method
hvap	109.30	kJ/mol	Joback Method
log10ws	-14.45		Crippen Method
logp	13.609		Crippen Method
mcvol	549.420	ml/mol	McGowan Method
pc	439.87	kPa	Joback Method
rinpol	3922.41		NIST Webbook
rinpol	3922.41		NIST Webbook
tb	1149.29	K	Joback Method
tc	1523.64	K	Joback Method
tf	585.10	K	Joback Method
vc	2.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2064.62	J/molxK	1149.29	Joback Method
cpg	2102.17	J/molxK	1211.68	Joback Method
cpg	2136.19	J/molxK	1274.07	Joback Method
cpg	2167.30	J/molxK	1336.46	Joback Method

cpg	2196.10	J/molxK	1398.86	Joback Method
cpg	2223.22	J/molxK	1461.25	Joback Method
cpg	2249.29	J/molxK	1523.64	Joback Method
dvisc	0.0001421	Paxs	585.10	Joback Method
dvisc	0.0000522	Paxs	679.13	Joback Method
dvisc	0.0000245	Paxs	773.16	Joback Method
dvisc	0.0000135	Paxs	867.19	Joback Method
dvisc	0.0000084	Paxs	961.23	Joback Method
dvisc	0.0000057	Paxs	1055.26	Joback Method
dvisc	0.0000041	Paxs	1149.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22393960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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