Octadec-9-enoic acid octadeca-9,12,15-trienyl ester, Z,Z,Z,Z

Inchi: InChI=1S/C36H64O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-
InchiKey: AGAGKLWHIZXMOT-UJGICNFHSA-N
Formula: C36H64O2
SMILES: CCC=CCC=CCC=CCCCCCCCCOC(=O)CCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 528.89

Physical Properties

Property code	Value	Unit	Source
gf	339.20	kJ/mol	Joback Method
hf	-562.29	kJ/mol	Joback Method
hfus	92.59	kJ/mol	Joback Method
hvap	104.72	kJ/mol	Joback Method
log10ws	-13.17		Crippen Method
logp	12.157		Crippen Method
mcvol	508.340	ml/mol	McGowan Method
pc	511.87	kPa	Joback Method
rinpol	3699.58		NIST Webbook
rinpol	3699.58		NIST Webbook
tb	1116.01	K	Joback Method
tc	1420.29	K	Joback Method
tf	547.32	K	Joback Method
vc	1.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1844.08	J/mol×K	1116.01	Joback Method
cpg	1877.03	J/mol×K	1166.72	Joback Method
cpg	1908.75	J/mol×K	1217.44	Joback Method
cpg	1939.65	J/mol×K	1268.15	Joback Method
cpg	1970.18	J/mol×K	1318.87	Joback Method
cpg	2000.75	J/mol×K	1369.58	Joback Method
cpg	2031.78	J/mol×K	1420.29	Joback Method
dvisc	0.0001575	Pa×s	547.32	Joback Method

dvisc	0.0000539	Pa×s	642.10	Joback Method
dvisc	0.0000243	Pa×s	736.88	Joback Method
dvisc	0.0000132	Pa×s	831.66	Joback Method
dvisc	0.0000081	Pa×s	926.45	Joback Method
dvisc	0.0000054	Pa×s	1021.23	Joback Method
dvisc	0.0000039	Pa×s	1116.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437220&Units=SI
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

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