Octadec-9-enoic acid octadeca-9,12-dienyl ester, Z,Z,Z

Inchi: InChI=1S/C36H66O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-
InchiKey: UHMXMURYWVGQFV-ZYYOPQBWSA-N
Formula: C36H66O2
SMILES: CCCCCC=CCC=CCCCCCCCCOC(=O)CCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 530.91

Physical Properties

Property code	Value	Unit	Source
gf	258.98	kJ/mol	Joback Method
hf	-679.51	kJ/mol	Joback Method
hfus	92.39	kJ/mol	Joback Method
hvap	104.76	kJ/mol	Joback Method
log10ws	-13.32		Crippen Method
logp	12.381		Crippen Method
mcvol	512.640	ml/mol	McGowan Method
pc	500.03	kPa	Joback Method
rinpol	3691.23		NIST Webbook
rinpol	3691.23		NIST Webbook
tb	1111.85	K	Joback Method
tc	1422.92	K	Joback Method
tf	552.40	K	Joback Method
vc	2.015	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1871.70	J/mol×K	1111.85	Joback Method
cpg	1904.80	J/mol×K	1163.69	Joback Method
cpg	1936.13	J/mol×K	1215.54	Joback Method
cpg	1966.13	J/mol×K	1267.38	Joback Method
cpg	1995.21	J/mol×K	1319.23	Joback Method
cpg	2023.77	J/mol×K	1371.07	Joback Method
cpg	2052.24	J/mol×K	1422.92	Joback Method
dvisc	0.0001682	Pa×s	552.40	Joback Method

dvisc	0.0000592	Pa×s	645.64	Joback Method
dvisc	0.0000271	Pa×s	738.88	Joback Method
dvisc	0.0000148	Pa×s	832.12	Joback Method
dvisc	0.0000091	Pa×s	925.37	Joback Method
dvisc	0.0000061	Pa×s	1018.61	Joback Method
dvisc	0.0000044	Pa×s	1111.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437106&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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