Octadeca-9,12-dienoic acid octadeca-9,12,15-trienyl ester

Inchi: InChI=1S/C36H62O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-

InchiKey: PEZVBHOZBJVGTI-HDFPZQRPSA-N

Formula: C36H62O2

SMILES: CCC=CCC=CCC=CCCCCCCCCCOC(=O)CCCCCCCC=CCC=CCCCCC

Mol. weight [g/mol]: 526.88

Physical Properties

Property code	Value	Unit	Source
gf	419.42	kJ/mol	Joback Method
hf	-445.07	kJ/mol	Joback Method
hfus	92.79	kJ/mol	Joback Method
hvap	104.68	kJ/mol	Joback Method
log10ws	-13.02		Crippen Method
logp	11.933		Crippen Method
mcvol	504.040	ml/mol	McGowan Method
pc	524.12	kPa	Joback Method
rinpol	3694.05		NIST Webbook
tb	1120.17	K	Joback Method
tc	1418.22	K	Joback Method
tf	542.24	K	Joback Method
vc	1.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1816.54	J/mol×K	1120.17	Joback Method
cpg	1977.85	J/mol×K	1368.54	Joback Method
cpg	1945.35	J/mol×K	1318.87	Joback Method
cpg	1913.40	J/mol×K	1269.19	Joback Method
cpg	1881.58	J/mol×K	1219.52	Joback Method
cpg	1849.43	J/mol×K	1169.84	Joback Method
cpg	2011.33	J/mol×K	1418.22	Joback Method
dvisc	0.0000034	Pa×s	1120.17	Joback Method
dvisc	0.0000048	Pa×s	1023.85	Joback Method

dvisc	0.0000072	Pa×s	927.53	Joback Method
dvisc	0.0000117	Pa×s	831.21	Joback Method
dvisc	0.0000218	Pa×s	734.88	Joback Method
dvisc	0.0000491	Pa×s	638.56	Joback Method
dvisc	0.0001475	Pa×s	542.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437235&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