Hexadecanoic acid octadeca-9,12-dienyl ester, Z

Inchi: InChI=1S/C34H64O2/c1-3-5-7-9-11-13-15-17-18-19-21-23-25-27-29-31-33-36-34(35)32-

InchiKey: FRGROTDLFLPWAC-XZBBILGWSA-N

Formula: C34H64O2

SMILES: CCCCCC=CCC=CCCCCCCCCOC(=O)CCCCCCCCCCCCCCC

Mol. weight [g/mol]: 504.87

Physical Properties

Property code	Value	Unit	Source
gf	161.92	kJ/mol	Joback Method
hf	-755.45	kJ/mol	Joback Method
hfus	87.01	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-12.62		Crippen Method
logp	11.824		Crippen Method
mcvol	488.760	ml/mol	McGowan Method
pc	532.87	kPa	Joback Method
rinpol	3516.49		NIST Webbook
rinpol	3516.49		NIST Webbook
tb	1061.93	K	Joback Method
tc	1343.48	K	Joback Method
tf	534.94	K	Joback Method
vc	1.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1762.72	J/mol×K	1061.93	Joback Method
cpg	1792.61	J/mol×K	1108.85	Joback Method
cpg	1820.51	J/mol×K	1155.78	Joback Method
cpg	1846.68	J/mol×K	1202.70	Joback Method
cpg	1871.38	J/mol×K	1249.63	Joback Method
cpg	1894.89	J/mol×K	1296.55	Joback Method
cpg	1917.46	J/mol×K	1343.48	Joback Method
dvisc	0.0002416	Pa×s	534.94	Joback Method

dvisc	0.0000880	Pa×s	622.77	Joback Method
dvisc	0.0000411	Pa×s	710.60	Joback Method
dvisc	0.0000227	Pa×s	798.43	Joback Method
dvisc	0.0000141	Pa×s	886.27	Joback Method
dvisc	0.0000096	Pa×s	974.10	Joback Method
dvisc	0.0000069	Pa×s	1061.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437077&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