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

Inchi: InChI=1S/C36H60O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-

InchiKey: LZUIYJJRANHRNH-XROYEESUSA-N

Formula: C36H60O2

SMILES: CCC=CCC=CCC=CCCCCCCCCOC(=O)CCCCCCCC=CCC=CCC=CCC

Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	499.64	kJ/mol	Joback Method
hf	-327.85	kJ/mol	Joback Method
hfus	93.00	kJ/mol	Joback Method
hvap	104.63	kJ/mol	Joback Method
log10ws	-12.88		Crippen Method
logp	11.709		Crippen Method
mcvol	499.740	ml/mol	McGowan Method
pc	536.83	kPa	Joback Method
rinpol	3702.13		NIST Webbook
tb	1124.33	K	Joback Method
tc	1416.67	K	Joback Method
tf	537.16	K	Joback Method
vc	1.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1789.07	J/mol×K	1124.33	Joback Method
cpg	1822.00	J/mol×K	1173.05	Joback Method
cpg	1854.64	J/mol×K	1221.78	Joback Method
cpg	1887.41	J/mol×K	1270.50	Joback Method
cpg	1920.77	J/mol×K	1319.23	Joback Method
cpg	1955.16	J/mol×K	1367.95	Joback Method
cpg	1991.01	J/mol×K	1416.67	Joback Method
dvisc	0.0001381	Pa×s	537.16	Joback Method
dvisc	0.0000448	Pa×s	635.02	Joback Method

dvisc	0.0000196	Pa×s	732.88	Joback Method
dvisc	0.0000104	Pa×s	830.74	Joback Method
dvisc	0.0000063	Pa×s	928.61	Joback Method
dvisc	0.0000042	Pa×s	1026.47	Joback Method
dvisc	0.0000030	Pa×s	1124.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437240&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