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

Inchi: InChI=1S/C32H56O2/c1-3-5-7-9-11-13-15-16-17-18-19-21-23-25-27-29-31-34-32(33)30-

InchiKey: QAEGREPHWCDXPX-ZBSLVJSLSA-N

Formula: C32H56O2

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

Mol. weight [g/mol]: 472.79

Physical Properties

Property code	Value	Unit	Source
gf	305.52	kJ/mol	Joback Method
hf	-479.73	kJ/mol	Joback Method
hfus	82.23	kJ/mol	Joback Method
hvap	95.81	kJ/mol	Joback Method
log10ws	-11.49		Crippen Method
logp	10.596		Crippen Method
mcvol	451.980	ml/mol	McGowan Method
pc	613.90	kPa	Joback Method
rinpol	3315.81		NIST Webbook
rinpol	3315.81		NIST Webbook
tb	1024.49	K	Joback Method
tc	1270.00	K	Joback Method
tf	502.24	K	Joback Method
vc	1.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1571.68	J/mol×K	1024.49	Joback Method
cpg	1597.77	J/mol×K	1065.41	Joback Method
cpg	1622.73	J/mol×K	1106.33	Joback Method
cpg	1646.75	J/mol×K	1147.24	Joback Method
cpg	1670.05	J/mol×K	1188.16	Joback Method
cpg	1692.82	J/mol×K	1229.08	Joback Method
cpg	1715.27	J/mol×K	1270.00	Joback Method
dvisc	0.0002828	Pa×s	502.24	Joback Method

dvisc	0.0000982	Pa×s	589.28	Joback Method
dvisc	0.0000448	Pa×s	676.32	Joback Method
dvisc	0.0000244	Pa×s	763.37	Joback Method
dvisc	0.0000151	Pa×s	850.41	Joback Method
dvisc	0.0000102	Pa×s	937.45	Joback Method
dvisc	0.0000073	Pa×s	1024.49	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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