Octadeca-9,12,15-trienoic acid hexadec-7-enyl ester, Z,Z,Z,Z

Inchi: InChI=1S/C34H60O2/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34(35)36-33-31-
InchiKey: ZZMQTBJTUVDBDO-PLNKFGNASA-N
Formula: C34H60O2
SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 500.84

Physical Properties

Property code	Value	Unit	Source
gf	322.36	kJ/mol	Joback Method
hf	-521.01	kJ/mol	Joback Method
hfus	87.41	kJ/mol	Joback Method
hvap	100.27	kJ/mol	Joback Method
log10ws	-12.33		Crippen Method
logp	11.376		Crippen Method
mcvol	480.160	ml/mol	McGowan Method
pc	559.41	kPa	Joback Method
rinpol	3504.89		NIST Webbook
rinpol	3504.89		NIST Webbook
tb	1070.25	K	Joback Method
tc	1341.75	K	Joback Method
tf	524.78	K	Joback Method
vc	1.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1706.86	J/mol×K	1070.25	Joback Method
cpg	1735.97	J/mol×K	1115.50	Joback Method
cpg	1763.87	J/mol×K	1160.75	Joback Method
cpg	1790.85	J/mol×K	1206.00	Joback Method
cpg	1817.21	J/mol×K	1251.25	Joback Method
cpg	1843.24	J/mol×K	1296.50	Joback Method
cpg	1869.21	J/mol×K	1341.75	Joback Method
dvisc	0.0002118	Pa×s	524.78	Joback Method

dvisc	0.0000730	Pa×s	615.69	Joback Method
dvisc	0.0000331	Pa×s	706.60	Joback Method
dvisc	0.0000180	Pa×s	797.51	Joback Method
dvisc	0.0000111	Pa×s	888.43	Joback Method
dvisc	0.0000074	Pa×s	979.34	Joback Method
dvisc	0.0000054	Pa×s	1070.25	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=R436821&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