Octadeca-9,12,15-trienoic acid tetradecyl ester,Z,Z,Z

Inchi: InChI=1S/C32H58O2/c1-3-5-7-9-11-13-15-17-18-19-20-22-24-26-28-30-32(33)34-31-29-

InchiKey: LNZYYCFZPLZOEF-SVNQLWEDSA-N

Formula: C32H58O2

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCC

Mol. weight [g/mol]: 474.80

Physical Properties

Property code	Value	Unit	Source
gf	225.30	kJ/mol	Joback Method
hf	-596.95	kJ/mol	Joback Method
hfus	82.03	kJ/mol	Joback Method
hvap	95.86	kJ/mol	Joback Method
log10ws	-11.64		Crippen Method
logp	10.820		Crippen Method
mcvol	456.280	ml/mol	McGowan Method
pc	598.38	kPa	Joback Method
rinpol	3322.43		NIST Webbook
rinpol	3322.43		NIST Webbook
tb	1020.33	K	Joback Method
tc	1268.87	K	Joback Method
tf	507.32	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1599.62	J/mol×K	1020.33	Joback Method
cpg	1626.17	J/mol×K	1061.75	Joback Method
cpg	1651.31	J/mol×K	1103.18	Joback Method
cpg	1675.22	J/mol×K	1144.60	Joback Method
cpg	1698.10	J/mol×K	1186.02	Joback Method
cpg	1720.15	J/mol×K	1227.44	Joback Method
cpg	1741.54	J/mol×K	1268.87	Joback Method
dvisc	0.0003019	Pa×s	507.32	Joback Method

dvisc	0.0001079	Pa×s	592.82	Joback Method
dvisc	0.0000499	Pa×s	678.32	Joback Method
dvisc	0.0000275	Pa×s	763.83	Joback Method
dvisc	0.0000171	Pa×s	849.33	Joback Method
dvisc	0.0000115	Pa×s	934.83	Joback Method
dvisc	0.0000083	Pa×s	1020.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436549&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