Icosa-5,8,11,14-tetraenoic acid tetradec-9-enyl ester

Inchi: InChI=1S/C34H58O2/c1-3-5-7-9-11-13-15-17-18-19-20-21-22-24-26-28-30-32-34(35)36-

InchiKey: WMEYKOAPDBHGDW-NXIMTCEVSA-N

Formula: C34H58O2

SMILES: CCCCC=CCCCCCCCCOC(=O)CCCC=CCC=CCC=CCC=CCCCCC

Mol. weight [g/mol]: 498.82

Physical Properties

Property code	Value	Unit	Source
gf	402.58	kJ/mol	Joback Method
hf	-403.79	kJ/mol	Joback Method
hfus	87.61	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-12.19		Crippen Method
logp	11.152		Crippen Method
mcvol	475.860	ml/mol	McGowan Method
pc	573.43	kPa	Joback Method
rinpol	3452.29		NIST Webbook
rinpol	3452.29		NIST Webbook
tb	1074.41	K	Joback Method
tc	1341.62	K	Joback Method
tf	519.70	K	Joback Method
vc	1.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1678.95	J/mol×K	1074.41	Joback Method
cpg	1707.81	J/mol×K	1118.95	Joback Method
cpg	1735.82	J/mol×K	1163.48	Joback Method
cpg	1763.29	J/mol×K	1208.02	Joback Method
cpg	1790.51	J/mol×K	1252.55	Joback Method
cpg	1817.78	J/mol×K	1297.09	Joback Method
cpg	1845.41	J/mol×K	1341.62	Joback Method
dvisc	0.0001984	Pa×s	519.70	Joback Method

dvisc	0.0000665	Pa×s	612.15	Joback Method
dvisc	0.0000297	Pa×s	704.60	Joback Method
dvisc	0.0000160	Pa×s	797.05	Joback Method
dvisc	0.0000098	Pa×s	889.51	Joback Method
dvisc	0.0000066	Pa×s	981.96	Joback Method
dvisc	0.0000047	Pa×s	1074.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436663&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