Octadeca-9,12-dienoic acid icosyl ester, Z

Inchi: InChI=1S/C38H72O2/c1-3-5-7-9-11-13-15-17-19-20-21-23-25-27-29-31-33-35-37-40-38(
InchiKey: FQZCMDHWPNQVQZ-GVKPZOCESA-N
Formula: C38H72O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 560.98

Physical Properties

Property code	Value	Unit	Source
gf	195.60	kJ/mol	Joback Method
hf	-838.01	kJ/mol	Joback Method
hfus	97.37	kJ/mol	Joback Method
hvap	109.25	kJ/mol	Joback Method
log10ws	-14.30		Crippen Method
logp	13.385		Crippen Method
mcvol	545.120	ml/mol	McGowan Method
pc	449.63	kPa	Joback Method
rinpol	3918.43		NIST Webbook
rinpol	3918.43		NIST Webbook
tb	1153.45	K	Joback Method
tc	1517.37	K	Joback Method
tf	580.02	K	Joback Method
vc	2.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2037.38	J/mol×K	1153.45	Joback Method
cpg	2074.96	J/mol×K	1214.10	Joback Method
cpg	2109.88	J/mol×K	1274.76	Joback Method
cpg	2142.76	J/mol×K	1335.41	Joback Method
cpg	2174.24	J/mol×K	1396.07	Joback Method
cpg	2204.95	J/mol×K	1456.72	Joback Method
cpg	2235.52	J/mol×K	1517.37	Joback Method
dvisc	0.0001329	Pa×s	580.02	Joback Method

dvisc	0.0000476	Pa×s	675.59	Joback Method
dvisc	0.0000220	Pa×s	771.16	Joback Method
dvisc	0.0000120	Pa×s	866.74	Joback Method
dvisc	0.0000074	Pa×s	962.31	Joback Method
dvisc	0.0000050	Pa×s	1057.88	Joback Method
dvisc	0.0000036	Pa×s	1153.45	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=R437304&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