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

Inchi: InChI=1S/C38H70O2/c1-3-5-7-9-11-13-15-17-19-20-21-23-25-27-29-31-33-35-37-40-38(

InchiKey: ZIFMUOBWYNUMBL-FLQWBAQUSA-N

Formula: C38H70O2

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

Mol. weight [g/mol]: 558.96

Physical Properties

Property code	Value	Unit	Source
gf	275.82	kJ/mol	Joback Method
hf	-720.79	kJ/mol	Joback Method
hfus	97.57	kJ/mol	Joback Method
hvap	109.21	kJ/mol	Joback Method
log10ws	-14.15		Crippen Method
logp	13.161		Crippen Method
mcvol	540.820	ml/mol	McGowan Method
pc	459.71	kPa	Joback Method
rinpol	3926.60		NIST Webbook
rinpol	3926.60		NIST Webbook
tb	1157.61	K	Joback Method
tc	1511.77	K	Joback Method
tf	574.94	K	Joback Method
vc	2.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2010.26	J/mol×K	1157.61	Joback Method
cpg	2186.29	J/mol×K	1452.75	Joback Method
cpg	2152.28	J/mol×K	1393.72	Joback Method
cpg	2118.31	J/mol×K	1334.69	Joback Method
cpg	2083.74	J/mol×K	1275.66	Joback Method
cpg	2047.94	J/mol×K	1216.64	Joback Method
cpg	2220.99	J/mol×K	1511.77	Joback Method
dvisc	0.0000032	Pa×s	1157.61	Joback Method

dvisc	0.0000044	Pa×s	1060.50	Joback Method
dvisc	0.0000066	Pa×s	963.39	Joback Method
dvisc	0.0000107	Pa×s	866.28	Joback Method
dvisc	0.0000198	Pa×s	769.16	Joback Method
dvisc	0.0000434	Pa×s	672.05	Joback Method
dvisc	0.0001243	Pa×s	574.94	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=R437319&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

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