Icosa-5,8,11,14-tetraenoic acid octadeca-9,12-dienyl ester

Inchi: InChI=1S/C38H64O2/c1-3-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-36-38(39)40-

InchiKey: BMVIOBOTDSTLAP-CEJABHJLSA-N

Formula: C38H64O2

SMILES: CCCCCC=CCC=CCC=CCC=CCCCC(=O)OCCCCCCCCC=CCC=CCCCCC

Mol. weight [g/mol]: 552.91

Physical Properties

Property code	Value	Unit	Source
gf	516.48	kJ/mol	Joback Method
hf	-369.13	kJ/mol	Joback Method
hfus	98.17	kJ/mol	Joback Method
hvap	109.09	kJ/mol	Joback Method
log10ws	-13.71		Crippen Method
logp	12.489		Crippen Method
mcvol	527.920	ml/mol	McGowan Method
pc	492.08	kPa	Joback Method
rinpol	3833.01		NIST Webbook
tb	1170.09	K	Joback Method
tc	1498.76	K	Joback Method
tf	559.70	K	Joback Method
vc	2.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1929.68	J/mol×K	1170.09	Joback Method
cpg	2129.25	J/mol×K	1443.98	Joback Method
cpg	2086.56	J/mol×K	1389.20	Joback Method
cpg	2045.90	J/mol×K	1334.42	Joback Method
cpg	2006.64	J/mol×K	1279.65	Joback Method
cpg	1968.12	J/mol×K	1224.87	Joback Method
cpg	2174.65	J/mol×K	1498.76	Joback Method
dvisc	0.0000022	Pa×s	1170.09	Joback Method
dvisc	0.0000031	Pa×s	1068.36	Joback Method

dvisc	0.0000046	Pa×s	966.63	Joback Method
dvisc	0.0000076	Pa×s	864.90	Joback Method
dvisc	0.0000144	Pa×s	763.16	Joback Method
dvisc	0.0000329	Pa×s	661.43	Joback Method
dvisc	0.0001020	Pa×s	559.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437146&Units=SI

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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