

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:	CCCCC=CCC=CC=CCC=CCCC(=O)OCCCCCCCCC=CCC=CCCCC
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/molxK	1170.09	Joback Method
cpg	1968.12	J/molxK	1224.87	Joback Method
cpg	2006.64	J/molxK	1279.65	Joback Method
cpg	2045.90	J/molxK	1334.42	Joback Method
cpg	2086.56	J/molxK	1389.20	Joback Method
cpg	2129.25	J/molxK	1443.98	Joback Method
cpg	2174.65	J/molxK	1498.76	Joback Method
dvisc	0.0001020	Paxs	559.70	Joback Method
dvisc	0.0000329	Paxs	661.43	Joback Method

dvisc	0.0000144	Paxs	763.16	Joback Method
dvisc	0.0000076	Paxs	864.90	Joback Method
dvisc	0.0000046	Paxs	966.63	Joback Method
dvisc	0.0000031	Paxs	1068.36	Joback Method
dvisc	0.0000022	Paxs	1170.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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