

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

Inchi:	InChI=1S/C38H66O2/c1-3-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-36-38(39)40-
InchiKey:	JHFDJRJMMSRXPU-WJNKXSRCSA-N
Formula:	C38H66O2
SMILES:	CCCCC=CCC=CC=CC=CCCC(=O)OCCCCCCCCC=CCCCCCCC
Mol. weight [g/mol]:	554.93

Physical Properties

Property code	Value	Unit	Source
gf	436.26	kJ/mol	Joback Method
hf	-486.35	kJ/mol	Joback Method
hfus	97.97	kJ/mol	Joback Method
hvap	109.13	kJ/mol	Joback Method
log10ws	-13.86		Crippen Method
logp	12.713		Crippen Method
mvol	532.220	ml/mol	McGowan Method
pc	480.92	kPa	Joback Method
rinpol	3837.23		NIST Webbook
rinpol	3837.23		NIST Webbook
tb	1165.93	K	Joback Method
tc	1502.48	K	Joback Method
tf	564.78	K	Joback Method
vc	2.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1956.40	J/molxK	1165.93	Joback Method
cpg	1994.51	J/molxK	1222.02	Joback Method
cpg	2032.10	J/molxK	1278.11	Joback Method
cpg	2069.84	J/molxK	1334.21	Joback Method
cpg	2108.36	J/molxK	1390.30	Joback Method
cpg	2148.33	J/molxK	1446.39	Joback Method
cpg	2190.38	J/molxK	1502.48	Joback Method
dvisc	0.0001089	Paxs	564.78	Joback Method

dvisc	0.0000361	Paxs	664.97	Joback Method
dvisc	0.0000160	Paxs	765.16	Joback Method
dvisc	0.0000085	Paxs	865.36	Joback Method
dvisc	0.0000052	Paxs	965.55	Joback Method
dvisc	0.0000035	Paxs	1065.74	Joback Method
dvisc	0.0000025	Paxs	1165.93	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=R437022&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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