Icosa-5,8,11,14-tetraenoic acid octadecyl ester, Z,Z,Z,Z

Inchi: InChI=1S/C38H68O2/c1-3-5-7-9-11-13-15-17-19-21-22-24-26-28-30-32-34-36-38(39)40-

InchiKey: INCGCRQVVSKVJP-LGHBDAFPSA-N

Formula: C38H68O2

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

Mol. weight [g/mol]: 556.95

Physical Properties

Property code	Value	Unit	Source
gf	356.04	kJ/mol	Joback Method
hf	-603.57	kJ/mol	Joback Method
hfus	97.77	kJ/mol	Joback Method
hvap	109.17	kJ/mol	Joback Method
log10ws	-14.01		Crippen Method
logp	12.937		Crippen Method
mcvol	536.520	ml/mol	McGowan Method
pc	470.13	kPa	Joback Method
rinpol	3863.07		NIST Webbook
rinpol	3863.07		NIST Webbook
tb	1161.77	K	Joback Method
tc	1506.82	K	Joback Method
tf	569.86	K	Joback Method
vc	2.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1983.26	J/mol×K	1161.77	Joback Method
cpg	2021.12	J/mol×K	1219.28	Joback Method
cpg	2057.81	J/mol×K	1276.79	Joback Method
cpg	2093.99	J/mol×K	1334.29	Joback Method
cpg	2130.29	J/mol×K	1391.80	Joback Method
cpg	2167.38	J/mol×K	1449.31	Joback Method
cpg	2205.89	J/mol×K	1506.82	Joback Method
dvisc	0.0001163	Pa×s	569.86	Joback Method

dvisc	0.0000396	Pa×s	668.51	Joback Method
dvisc	0.0000178	Pa×s	767.16	Joback Method
dvisc	0.0000096	Pa×s	865.81	Joback Method
dvisc	0.0000059	Pa×s	964.47	Joback Method
dvisc	0.0000039	Pa×s	1063.12	Joback Method
dvisc	0.0000028	Pa×s	1161.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436910&Units=SI
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

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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