9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Other names: Linolein, 2-mono-
«beta»-Monolinolein
(9Z,12Z)-1,3-Dihydroxypropan-2-yl octadeca-9,12-dienoate

Inchi: InChI=1S/C21H38O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-20(18-22)19

InchiKey: IEPGNWMPIFDNSD-HZJYTTRNSA-N

Formula: C21H38O4

SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OC(CO)CO

Mol. weight [g/mol]: 354.52

CAS: 3443-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-223.62	kJ/mol	Joback Method
hf	-796.87	kJ/mol	Joback Method
hfus	57.99	kJ/mol	Joback Method
hvap	104.38	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.696		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2706.90		NIST Webbook
rinpol	2706.90		NIST Webbook
tb	948.41	K	Joback Method
tc	1167.58	K	Joback Method
tf	495.07	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.94	J/mol×K	948.41	Joback Method
cpg	1080.16	J/mol×K	984.94	Joback Method
cpg	1096.40	J/mol×K	1021.47	Joback Method
cpg	1111.75	J/mol×K	1057.99	Joback Method

cpg	1126.28	J/mol×K	1094.52	Joback Method
cpg	1140.09	J/mol×K	1131.05	Joback Method
cpg	1153.26	J/mol×K	1167.58	Joback Method
dvisc	0.0002816	Pa×s	495.07	Joback Method
dvisc	0.0000553	Pa×s	570.63	Joback Method
dvisc	0.0000159	Pa×s	646.18	Joback Method
dvisc	0.0000059	Pa×s	721.74	Joback Method
dvisc	0.0000027	Pa×s	797.30	Joback Method
dvisc	0.0000014	Pa×s	872.85	Joback Method
dvisc	0.0000008	Pa×s	948.41	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3443821&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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