9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-

Other names: 1,2,3-propanetriyl tris[(E)-9-octadecenoate]
trielaidin

Inchi: InChI=1S/C57H104O6/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-55(58)61-52-

InchiKey: PHYFQTYBJUILEZ-WUOFIQDXSA-N

Formula: C57H104O6

SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC=CCCCCCCCC)OC(=O)

Mol. weight [g/mol]: 885.43

CAS: 537-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.48	kJ/mol	Joback Method
hf	-1607.83	kJ/mol	Joback Method
hfus	157.08	kJ/mol	Investigation of the Thermal Behaviour of Trielaidin Between 10 K and 360 K
hvap	169.43	kJ/mol	Joback Method
log10ws	-19.94		Crippen Method
logp	18.097		Crippen Method
mcvol	823.410	ml/mol	McGowan Method
pc	245.06	kPa	Joback Method
tb	1744.47	K	Joback Method
tc	4418.33	K	Joback Method
tf	918.39	K	Joback Method
vc	3.233	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3418.56	J/mol×K	1744.47	Joback Method
cpg	3789.05	J/mol×K	2190.11	Joback Method
cpg	4601.71	J/mol×K	2635.76	Joback Method
cpg	6184.33	J/mol×K	3081.40	Joback Method
cpg	8864.70	J/mol×K	3527.04	Joback Method

cpg	12970.60	J/mol×K	3972.68	Joback Method
cpg	18829.83	J/mol×K	4418.33	Joback Method
dvisc	0.0000014	Pa×s	918.39	Joback Method
dvisc	0.0000006	Pa×s	1056.07	Joback Method
dvisc	0.0000003	Pa×s	1193.75	Joback Method
dvisc	0.0000001	Pa×s	1331.43	Joback Method
dvisc	9.1401528e-08	Pa×s	1469.11	Joback Method
dvisc	6.1659533e-08	Pa×s	1606.79	Joback Method
dvisc	4.4262050e-08	Pa×s	1744.47	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=C537393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Investigation of the Thermal Behaviour of Trielaidin Between 10 K and 360 K:	https://www.doi.org/10.1021/je034048e

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume