Octadecanoic acid, 1,3-propanediyl ester

Other names:	Stearic acid, trimethylene ester
	1,3-Di-O-octadecanoylpropanediol
	1,3-Propanediol, distearate
Inchi:	InChI=1S/C39H76O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-34-38(40)42-36-33-
InchiKey:	UFASAALQMYZBEM-UHFFFAOYSA-N
Formula:	C39H76O4
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCCCOC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	609.02
CAS:	17367-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-190.34	kJ/mol	Joback Method
hf	-1337.89	kJ/mol	Joback Method
hfus	102.34	kJ/mol	Joback Method
hvap	120.72	kJ/mol	Joback Method
log10ws	-13.87		Crippen Method
logp	12.986		Crippen Method
mcvol	575.250	ml/mol	McGowan Method
pc	421.64	kPa	Joback Method
tb	1244.30	K	Joback Method
tc	1736.77	K	Joback Method
tf	673.61	K	Joback Method
vc	2.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2316.22	J/mol×K	1736.77	Joback Method
cpg	2201.29	J/mol×K	1244.30	Joback Method
cpg	2235.18	J/mol×K	1326.38	Joback Method
cpg	2261.74	J/mol×K	1408.46	Joback Method
cpg	2282.04	J/mol×K	1490.54	Joback Method
cpg	2297.17	J/mol×K	1572.61	Joback Method

cpg	2308.21	J/mol×K	1654.69	Joback Method
dvisc	0.0000026	Pa×s	1244.30	Joback Method
dvisc	0.0000638	Pa×s	673.61	Joback Method
dvisc	0.0000268	Pa×s	768.73	Joback Method
dvisc	0.0000136	Pa×s	863.84	Joback Method
dvisc	0.0000079	Pa×s	958.95	Joback Method
dvisc	0.0000051	Pa×s	1054.07	Joback Method
dvisc	0.0000035	Pa×s	1149.18	Joback Method
hfust	110.00	kJ/mol	329.80	NIST Webbook

Sources

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=C17367441&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
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