1,2-Distearin

Other names: (±)-1-(hydroxymethyl)ethane-1,2-diyl distearate
Inchi: InChI=1S/C39H76O5/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-38(41)43-36-37(
InchiKey: UHUSDOQQWJGJQS-UHFFFAOYSA-N
Formula: C39H76O5
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(CO)OC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 625.02
CAS: 51063-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-329.60	kJ/mol	Joback Method
hf	-1495.40	kJ/mol	Joback Method
hfus	102.91	kJ/mol	Joback Method
hvap	137.01	kJ/mol	Joback Method
log10ws	-13.25		Crippen Method
logp	11.957		Crippen Method
mcvol	581.120	ml/mol	McGowan Method
pc	439.50	kPa	Joback Method
tb	1336.04	K	Joback Method
tc	2006.21	K	Joback Method
tf	719.43	K	Joback Method
vc	2.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2257.79	J/mol×K	1336.04	Joback Method
cpg	2348.95	J/mol×K	1894.52	Joback Method
cpg	2340.44	J/mol×K	1782.82	Joback Method
cpg	2329.87	J/mol×K	1671.13	Joback Method
cpg	2314.44	J/mol×K	1559.43	Joback Method
cpg	2291.34	J/mol×K	1447.74	Joback Method
cpg	2358.18	J/mol×K	2006.21	Joback Method
dvisc	0.0000002	Pa×s	1336.04	Joback Method

dvisc	0.0000003	Pa×s	1233.27	Joback Method
dvisc	0.0000005	Pa×s	1130.50	Joback Method
dvisc	0.0000008	Pa×s	1027.74	Joback Method
dvisc	0.0000017	Pa×s	924.97	Joback Method
dvisc	0.0000040	Pa×s	822.20	Joback Method
dvisc	0.0000123	Pa×s	719.43	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51063979&Units=SI

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