Alpha-stearoyl stearic acid, methyl ester

Inchi: InChI=1S/C37H72O3/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36(38)35(37(39
InchiKey: QSOSUDRRPSNGFF-UHFFFAOYSA-N
Formula: C37H72O3
SMILES: CCCCCCCCCCCCCCCCCC(=O)C(CCCCCCCCCCCCCCCCC)C(=O)OC
Mol. weight [g/mol]: 564.97
CAS: 10126-69-9

Physical Properties

Property code	Value	Unit	Source
gf	-104.62	kJ/mol	Joback Method
hf	-1169.67	kJ/mol	Joback Method
hfus	92.45	kJ/mol	Joback Method
hvap	113.47	kJ/mol	Joback Method
log10ws	-13.21		Crippen Method
logp	12.478		Crippen Method
mcvol	541.200	ml/mol	McGowan Method
pc	461.89	kPa	Joback Method
tb	1175.68	K	Joback Method
tc	1563.75	K	Joback Method
tf	613.84	K	Joback Method
vc	2.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2041.16	J/mol×K	1175.68	Joback Method
cpg	2167.88	J/mol×K	1499.07	Joback Method
cpg	2148.93	J/mol×K	1434.40	Joback Method
cpg	2127.36	J/mol×K	1369.72	Joback Method
cpg	2102.59	J/mol×K	1305.04	Joback Method
cpg	2074.05	J/mol×K	1240.36	Joback Method
cpg	2184.79	J/mol×K	1563.75	Joback Method
dvisc	0.0000045	Pa×s	1175.68	Joback Method
dvisc	0.0000063	Pa×s	1082.04	Joback Method

dvisc	0.0000092	Pa×s	988.40	Joback Method
dvisc	0.0000148	Pa×s	894.76	Joback Method
dvisc	0.0000265	Pa×s	801.12	Joback Method
dvisc	0.0000552	Pa×s	707.48	Joback Method
dvisc	0.0001439	Pa×s	613.84	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=C10126699&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