Octadecanoic acid, 2,3-bis(acetyloxy)propyl ester

Other names: Stearic acid, 2,3-dihydroxypropyl ester diacetate
2,3-Bis(acetyloxy)propyl stearate
Glycerol, 1-octadecanoate, diacetate
NSC 83201
1,2-Diaceto-3-stearin

Inchi: InChI=1S/C25H46O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-25(28)30-21-24(31

InchiKey: WSYNAKWAAXYNMW-UHFFFAOYSA-N

Formula: C25H46O6

SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(COC(C)=O)OC(C)=O

Mol. weight [g/mol]: 442.63

CAS: 33599-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-544.58	kJ/mol	Joback Method
hf	-1299.01	kJ/mol	Joback Method
hfus	65.34	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.286		Crippen Method
mcvol	385.430	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
tb	999.83	K	Joback Method
tc	1233.94	K	Joback Method
tf	572.99	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.11	J/mol×K	999.83	Joback Method
cpg	1350.36	J/mol×K	1038.85	Joback Method
cpg	1366.61	J/mol×K	1077.87	Joback Method
cpg	1380.90	J/mol×K	1116.88	Joback Method

cpg	1393.25	J/mol×K	1155.90	Joback Method
cpg	1403.71	J/mol×K	1194.92	Joback Method
cpg	1412.30	J/mol×K	1233.94	Joback Method
dvisc	0.0002679	Pa×s	572.99	Joback Method
dvisc	0.0001286	Pa×s	644.13	Joback Method
dvisc	0.0000714	Pa×s	715.27	Joback Method
dvisc	0.0000441	Pa×s	786.41	Joback Method
dvisc	0.0000295	Pa×s	857.55	Joback Method
dvisc	0.0000210	Pa×s	928.69	Joback Method
dvisc	0.0000157	Pa×s	999.83	Joback Method
hfust	45.56	kJ/mol	208.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33599074&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
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