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

Other names: Glycerol, 1-hexadecanoate, diacetate
Inchi: InChI=1S/C23H42O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23(26)28-19-22(29-21(3)2
InchiKey: CIUYPOUJRYWLDF-UHFFFAOYSA-N
Formula: C23H42O6
SMILES: CCCCCCCCCCCCCCCC(=O)OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 414.58
CAS: 55268-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-561.42	kJ/mol	Joback Method
hf	-1257.73	kJ/mol	Joback Method
hfus	60.16	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.506		Crippen Method
mcvol	357.250	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
tb	954.07	K	Joback Method
tc	1170.70	K	Joback Method
tf	550.45	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.03	J/mol×K	954.07	Joback Method
cpg	1278.29	J/mol×K	1134.59	Joback Method
cpg	1267.25	J/mol×K	1098.49	Joback Method
cpg	1254.63	J/mol×K	1062.38	Joback Method
cpg	1240.40	J/mol×K	1026.28	Joback Method
cpg	1224.54	J/mol×K	990.17	Joback Method
cpg	1287.75	J/mol×K	1170.70	Joback Method
dvisc	0.0000216	Pa×s	954.07	Joback Method

dvisc	0.0000288	Pa×s	886.80	Joback Method
dvisc	0.0000402	Pa×s	819.53	Joback Method
dvisc	0.0000597	Pa×s	752.26	Joback Method
dvisc	0.0000958	Pa×s	684.99	Joback Method
dvisc	0.0001702	Pa×s	617.72	Joback Method
dvisc	0.0003483	Pa×s	550.45	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=C55268707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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