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

Other names: 2,3-Bis(acetyloxy)propyl dodecanoate
Propyl dodecanoic acid, 2,3-bis(acetyloxy)
Inchi: InChI=1S/C19H34O6/c1-4-5-6-7-8-9-10-11-12-13-19(22)24-15-18(25-17(3)21)14-23-16(2
InchiKey: NBMAHNZMRSQCPG-UHFFFAOYSA-N
Formula: C19H34O6
SMILES: CCCCCCCCCCCC(=O)OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 358.47
CAS: 55191-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-595.10	kJ/mol	Joback Method
hf	-1175.17	kJ/mol	Joback Method
hfus	49.80	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.945		Crippen Method
mcvol	300.890	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
tb	862.55	K	Joback Method
tc	1057.38	K	Joback Method
tf	505.37	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.35	J/mol×K	862.55	Joback Method
cpg	978.50	J/mol×K	895.02	Joback Method
cpg	993.48	J/mol×K	927.49	Joback Method
cpg	1007.27	J/mol×K	959.96	Joback Method
cpg	1019.88	J/mol×K	992.44	Joback Method
cpg	1031.32	J/mol×K	1024.91	Joback Method
cpg	1041.60	J/mol×K	1057.38	Joback Method

dvisc	0.0005695	Pa×s	505.37	Joback Method
dvisc	0.0002897	Pa×s	564.90	Joback Method
dvisc	0.0001676	Pa×s	624.43	Joback Method
dvisc	0.0001067	Pa×s	683.96	Joback Method
dvisc	0.0000730	Pa×s	743.49	Joback Method
dvisc	0.0000528	Pa×s	803.02	Joback Method
dvisc	0.0000400	Pa×s	862.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191441&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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