9-Octadecenoic acid (Z)-, 2,3-bis(acetyloxy)propyl ester

Other names: Glyceryl 1-oleate, diacetate

1-Oleoyl-2,3-diacetyl-glycerol

Inchi: InChI=1S/C25H44O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-25(28)30-21-24(31

InchiKey: KXLSJQTXSAYFDL-QXMHVHEDSA-N

Formula: C25H44O6

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

Mol. weight [g/mol]: 440.61

CAS: 55401-64-4

Physical Properties

Property code	Value	Unit	Source
gf	-464.36	kJ/mol	Joback Method
hf	-1181.79	kJ/mol	Joback Method
hfus	65.55	kJ/mol	Joback Method
hvap	98.28	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.062		Crippen Method
mcvol	381.130	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	1003.99	K	Joback Method
tc	1236.33	K	Joback Method
tf	567.91	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1303.55	J/mol×K	1003.99	Joback Method
cpg	1321.36	J/mol×K	1042.71	Joback Method
cpg	1337.39	J/mol×K	1081.44	Joback Method
cpg	1351.71	J/mol×K	1120.16	Joback Method
cpg	1364.34	J/mol×K	1158.88	Joback Method
cpg	1375.36	J/mol×K	1197.61	Joback Method

cpg	1384.80	J/mol×K	1236.33	Joback Method
dvisc	0.0002490	Pa×s	567.91	Joback Method
dvisc	0.0001169	Pa×s	640.59	Joback Method
dvisc	0.0000641	Pa×s	713.27	Joback Method
dvisc	0.0000392	Pa×s	785.95	Joback Method
dvisc	0.0000261	Pa×s	858.63	Joback Method
dvisc	0.0000185	Pa×s	931.31	Joback Method
dvisc	0.0000138	Pa×s	1003.99	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=C55401644&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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