

2-Methoxyethyl (9z)-12-(acetyloxy)-9-octadecenoate

Other names:	2-methoxyethyl (R)-12-(acetoxy)oleate
Inchi:	InChI=1S/C23H42O5/c1-4-5-6-13-16-22(28-21(2)24)17-14-11-9-7-8-10-12-15-18-23(25)2
InchiKey:	BJJRVZBBFAXWGR-KAMYIIQDSA-N
Formula:	C23H42O5
SMILES:	CCCCCCCC(CC=CCCCCCCCC(=O)OCCOC)OC(C)=O
Mol. weight [g/mol]:	398.58
CAS:	140-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-352.28	kJ/mol	Joback Method
hf	-1027.93	kJ/mol	Joback Method
hfus	58.77	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.755		Crippen Method
mcvol	351.380	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
tb	904.36	K	Joback Method
tc	1107.38	K	Joback Method
tf	495.44	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.97	J/mol×K	904.36	Joback Method
cpg	1178.69	J/mol×K	938.20	Joback Method
cpg	1196.05	J/mol×K	972.03	Joback Method
cpg	1212.11	J/mol×K	1005.87	Joback Method
cpg	1226.88	J/mol×K	1039.71	Joback Method
cpg	1240.39	J/mol×K	1073.55	Joback Method
cpg	1252.68	J/mol×K	1107.38	Joback Method
dvisc	0.0004300	Pa×s	495.44	Joback Method

dvisc	0.0001899	Pa×s	563.59	Joback Method
dvisc	0.0001000	Pa×s	631.75	Joback Method
dvisc	0.0000597	Pa×s	699.90	Joback Method
dvisc	0.0000390	Pa×s	768.05	Joback Method
dvisc	0.0000274	Pa×s	836.21	Joback Method
dvisc	0.0000202	Pa×s	904.36	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=C140056&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

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