

Dodecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester

Other names:

2-(Acetyloxy)-1-[(acetyloxy)methyl]ethyl dodecanoate

Ethyl dodecanoic acid, 2-(acetyloxy)-1-((acetyloxy)methyl)

Inchi: InChI=1S/C19H34O6/c1-4-5-6-7-8-9-10-11-12-13-19(22)25-18(14-23-16(2)20)15-24-17(3)

InchiKey: IADBTKCAYVABOP-UHFFFAOYSA-N

Formula: C19H34O6

SMILES: CCCCCCCCCC(=O)OC(COC(C)=O)COC(C)=O

Mol. weight [g/mol]: 358.47

CAS: 55191-43-0

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
mvol	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	m ³ /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	Paxs	505.37	Joback Method
dvisc	0.0002897	Paxs	564.90	Joback Method
dvisc	0.0001676	Paxs	624.43	Joback Method
dvisc	0.0001067	Paxs	683.96	Joback Method
dvisc	0.0000730	Paxs	743.49	Joback Method
dvisc	0.0000528	Paxs	803.02	Joback Method
dvisc	0.0000400	Paxs	862.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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