Acetic acid 2-ethoxymethyl-4,5-dimethoxy-tetrahydro-pyran-3-ester

Inchi: InChI=1S/C12H22O6/c1-5-16-6-10-12(18-8(2)13)11(15-4)9(14-3)7-17-10/h9-12H,5-7H2,

InchiKey: LSKFOPUESJEQHM-UHFFFAOYSA-N

Formula: C12H22O6

SMILES: CCOCC1OCC(OC)C(OC)C1OC(C)=O

Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-583.56	kJ/mol	Joback Method
hf	-1071.17	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	62.70	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.383		Crippen Method
mcvol	200.000	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1594.56		NIST Webbook
rinpol	1586.92		NIST Webbook
rinpol	1571.51		NIST Webbook
tb	650.00	K	Joback Method
tc	843.28	K	Joback Method
tf	385.08	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.70	J/mol×K	650.00	Joback Method
cpg	662.58	J/mol×K	811.07	Joback Method
cpg	647.96	J/mol×K	778.86	Joback Method
cpg	632.32	J/mol×K	746.64	Joback Method
cpg	615.71	J/mol×K	714.43	Joback Method
cpg	598.16	J/mol×K	682.21	Joback Method
cpg	676.15	J/mol×K	843.28	Joback Method

dvisc	0.0001501	Pa×s	650.00	Joback Method
dvisc	0.0001833	Pa×s	605.85	Joback Method
dvisc	0.0002310	Pa×s	561.69	Joback Method
dvisc	0.0003028	Pa×s	517.54	Joback Method
dvisc	0.0004176	Pa×s	473.39	Joback Method
dvisc	0.0006152	Pa×s	429.23	Joback Method
dvisc	0.0009905	Pa×s	385.08	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=R262467&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