Acetic acid 3-acetoxy-5-methoxy-tetrahydro-pyran-4-yl ester

Inchi: InChI=1S/C10H16O6/c1-6(11)15-9-5-14-4-8(13-3)10(9)16-7(2)12/h8-10H,4-5H2,1-3H3
InchiKey: MVVNLUDKWSGDPL-UHFFFAOYSA-N
Formula: C10H16O6
SMILES: COC1COCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 232.23

Physical Properties

Property code	Value	Unit	Source
gf	-616.61	kJ/mol	Joback Method
hf	-989.91	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.105		Crippen Method
mcvol	167.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1443.72		NIST Webbook
rinpol	1443.72		NIST Webbook
tb	640.36	K	Joback Method
tc	847.49	K	Joback Method
tf	394.48	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.79	J/mol×K	640.36	Joback Method
cpg	482.87	J/mol×K	674.88	Joback Method
cpg	498.07	J/mol×K	709.40	Joback Method
cpg	512.36	J/mol×K	743.92	Joback Method
cpg	525.70	J/mol×K	778.44	Joback Method
cpg	538.07	J/mol×K	812.97	Joback Method
cpg	549.43	J/mol×K	847.49	Joback Method
dvisc	0.0013874	Pa×s	394.48	Joback Method

dvisc	0.0008679	Pa×s	435.46	Joback Method
dvisc	0.0005885	Pa×s	476.44	Joback Method
dvisc	0.0004244	Pa×s	517.42	Joback Method
dvisc	0.0003211	Pa×s	558.40	Joback Method
dvisc	0.0002524	Pa×s	599.38	Joback Method
dvisc	0.0002046	Pa×s	640.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R268118&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

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