Acetic acid 3-acetoxy-2-acetoxymethyl-5-(acetyl-methyl-amin ester

Inchi: InChI=1S/C16H25NO9/c1-8(18)17(5)13-15(25-11(4)21)14(24-10(3)20)12(7-23-9(2)19)26
InchiKey: YHVKYAZUIGOUHQ-UHFFFAOYSA-N
Formula: C16H25NO9
SMILES: COC1OC(COC(C)=O)C(OC(C)=O)C(OC(C)=O)C1N(C)C(C)=O
Mol. weight [g/mol]: 375.37

Physical Properties

Property code	Value	Unit	Source
gf	-833.57	kJ/mol	Joback Method
hf	-1444.28	kJ/mol	Joback Method
hfus	55.46	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-0.58		Crippen Method
logp	-0.369		Crippen Method
mcvol	271.050	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2197.34		NIST Webbook
tb	910.90	K	Joback Method
tc	1122.34	K	Joback Method
tf	608.18	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.10	J/mol×K	910.90	Joback Method
cpg	927.34	J/mol×K	946.14	Joback Method
cpg	938.80	J/mol×K	981.38	Joback Method
cpg	948.44	J/mol×K	1016.62	Joback Method
cpg	956.24	J/mol×K	1051.86	Joback Method
cpg	962.14	J/mol×K	1087.10	Joback Method
cpg	966.12	J/mol×K	1122.34	Joback Method

Sources

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=R500888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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