Acetic acid 5-(acetyl-methyl-amino) -4,6-dimethoxy-2-methoxymethyl-tetrahydro-pyra ester

Inchi: InChI=1S/C14H25NO7/c1-8(16)15(3)11-13(19-5)12(21-9(2)17)10(7-18-4)22-14(11)20-6/h10-14H,7H2,1-6H3/t10-,11-,12-,13-,14?/m1/s1

InchiKey: VECKDHFNGOJJAQ-UHFFFAOYSA-N

Formula: C14H25NO7

SMILES: COCC1OC(OC)C(N(C)C(C)=O)C(OC)C1OC(C)=O

Mol. weight [g/mol]: 319.35

Physical Properties

Property code	Value	Unit	Source
gf	-592.57	kJ/mol	Joback Method
hf	-1177.84	kJ/mol	Joback Method
hfus	47.08	kJ/mol	Joback Method
hvap	75.64	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	-0.202		Crippen Method
mcvol	239.730	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1971.01		NIST Webbook
rinpol	1971.01		NIST Webbook
tb	757.40	K	Joback Method
tc	952.86	K	Joback Method
tf	485.78	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.86	J/mol×K	757.40	Joback Method
cpg	778.75	J/mol×K	789.98	Joback Method
cpg	795.41	J/mol×K	822.55	Joback Method
cpg	810.79	J/mol×K	855.13	Joback Method
cpg	824.86	J/mol×K	887.70	Joback Method
cpg	837.59	J/mol×K	920.28	Joback Method
cpg	848.95	J/mol×K	952.86	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=R500917&Units=SI

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