

Acetic acid 5-(acetyl-methyl-amino)-3,4,6-trimethoxy-tetrahydro-pyran-2-ylmethyl ester

Inchi:
InchiKey:

InChI=1S/C14H25NO7/c1-8(16)15(3)11-13(19-5)12(18-4)10(7-21-9(2)17)22-14(11)20-6/

OJKWAYQEHPUNL-UHFFFAOYSA-N

Formula:

C14H25NO7

SMILES:

COC1OC(COC(C)=O)C(OC)C(OC)C1N(C)C(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	1983.04		NIST Webbook
rinpol	1983.04		NIST Webbook
tb	757.40	K	Joback Method
tc	952.86	K	Joback Method
tf	485.78	K	Joback Method
vc	0.872	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.86	J/molxK	757.40	Joback Method
cpg	778.75	J/molxK	789.98	Joback Method
cpg	795.41	J/molxK	822.55	Joback Method
cpg	810.79	J/molxK	855.13	Joback Method
cpg	824.86	J/molxK	887.70	Joback Method
cpg	837.59	J/molxK	920.28	Joback Method
cpg	848.95	J/molxK	952.86	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=R194760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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