Methyl 4,6-di-O-acetyl-2-deoxy-3-O-methyl-2-(N-methylac

Other names: Acetic acid 2-acetoxymethyl-5-(acetyl-methyl-amino)-4,6-dimethoxy-tetrahydro-pyran-3-yl ester

Inchi: InChI=1S/C15H25NO8/c1-8(17)16(4)12-14(20-5)13(23-10(3)19)11(7-22-9(2)18)24-15(12

InchiKey: KVHWXZLZEULMLF-YYFQZIEXSA-N

Formula: C15H25NO8

SMILES: COC1OC(COC(C)=O)C(OC(C)=O)C(OC)C1N(C)C(C)=O

Mol. weight [g/mol]: 347.36

CAS: 56341-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-713.07	kJ/mol	Joback Method
hf	-1311.06	kJ/mol	Joback Method
hfus	51.27	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.286		Crippen Method
mcvol	255.390	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2109.46		NIST Webbook
rinpol	2109.46		NIST Webbook
tb	834.15	K	Joback Method
tc	1036.62	K	Joback Method
tf	546.98	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.19	J/mol×K	834.15	Joback Method
cpg	856.04	J/mol×K	867.89	Joback Method
cpg	870.40	J/mol×K	901.64	Joback Method
cpg	883.26	J/mol×K	935.38	Joback Method
cpg	894.56	J/mol×K	969.13	Joback Method
cpg	904.28	J/mol×K	1002.87	Joback Method

cpg	912.37	J/mol×K	1036.62	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=C56341516&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