

Methyl 2-deoxy-3,4,6-tri-O-methyl-2-(N-methylacetamido)

Inchi:	InChI=1S/C13H25NO6/c1-8(15)14(2)10-12(18-5)11(17-4)9(7-16-3)20-13(10)19-6/h9-13H
InchiKey:	LLBFFWSIFJDSHK-PPCPHDFISA-N
Formula:	C13H25NO6
SMILES:	COCC1OC(OC)C(N(C)C(C)=O)C(OC)C1OC
Mol. weight [g/mol]:	291.34

Physical Properties

Property code	Value	Unit	Source
gf	-472.07	kJ/mol	Joback Method
hf	-1044.62	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	5.01e-03		Crippen Method
logp	-0.119		Crippen Method
mcvol	224.070	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1869.61		NIST Webbook
rinpol	1869.61		NIST Webbook
tb	680.65	K	Joback Method
tc	870.20	K	Joback Method
tf	424.58	K	Joback Method
vc	0.809	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.56	J/molxK	680.65	Joback Method
cpg	696.96	J/molxK	712.24	Joback Method
cpg	715.33	J/molxK	743.83	Joback Method
cpg	732.64	J/molxK	775.43	Joback Method
cpg	748.85	J/molxK	807.02	Joback Method
cpg	763.93	J/molxK	838.61	Joback Method
cpg	777.86	J/molxK	870.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R391585&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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