

4-Acetoxy-3,6-dimethoxy-5-[2-(N-methyl-acetamid

Inchi:	InChI=1S/C23H25NO5/c1-14(25)24(3)13-12-18-19(27-4)10-8-16-6-7-17-9-11-20(28-5)23
InchiKey:	BNNUJMGLZXKERQ-UHFFFAOYSA-N
Formula:	C23H25NO5
SMILES:	<chem>COc1ccc2ccc3ccc(OC)c(OC(C)=O)c3c2c1CCN(C)C(C)=O</chem>
Mol. weight [g/mol]:	395.45

Physical Properties

Property code	Value	Unit	Source
gf	-41.72	kJ/mol	Joback Method
hf	-511.02	kJ/mol	Joback Method
hfus	51.24	kJ/mol	Joback Method
hvap	98.42	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	3.956		Crippen Method
mvol	302.980	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	3064.00		NIST Webbook
tb	1002.62	K	Joback Method
tc	1234.33	K	Joback Method
tf	702.41	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.10	J/molxK	1002.62	Joback Method
cpg	975.85	J/molxK	1041.24	Joback Method
cpg	987.48	J/molxK	1079.86	Joback Method
cpg	998.05	J/molxK	1118.48	Joback Method
cpg	1007.63	J/molxK	1157.10	Joback Method
cpg	1016.28	J/molxK	1195.71	Joback Method
cpg	1024.06	J/molxK	1234.33	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=R330773&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
mccvol:	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

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