4-Acetyloxy-3,6-dimethoxy-8-[2-(N-methyl-acetam

Inchi: InChI=1S/C23H25NO5/c1-14(25)24(3)11-10-17-12-18(27-4)13-20-19(17)8-6-16-7-9-21(2
InchiKey: IQCNMUAWZXTDNZ-UHFFFAOYSA-N
Formula: C23H25NO5
SMILES: COc1cc(CCN(C)C(C)=O)c2ccc3ccc(OC)c(OC(C)=O)c3c2c1
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
mcvol	302.980	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	3515.00		NIST Webbook
rinpol	3515.00		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/mol×K	1002.62	Joback Method
cpg	975.85	J/mol×K	1041.24	Joback Method
cpg	987.48	J/mol×K	1079.86	Joback Method
cpg	998.05	J/mol×K	1118.48	Joback Method
cpg	1007.63	J/mol×K	1157.10	Joback Method
cpg	1016.28	J/mol×K	1195.71	Joback Method
cpg	1024.06	J/mol×K	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=R330788&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