Acetamide, N-[2-[3,4-bis(acetyloxy)phenyl]-2-hydroxyethyl]-N

Other names: Acetamide, N-methyl-N-(beta,3,4-trihydroxyphenethyl)-, 3,4-diacetate
Inchi: InChI=1S/C15H19NO6/c1-9(17)16(4)8-13(20)12-5-6-14(21-10(2)18)15(7-12)22-11(3)19/
InchiKey: VIEBAWINIWTURC-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CC(=O)Oc1ccc(C(O)CN(C)C(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 309.31
CAS: 55712-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-456.67	kJ/mol	Joback Method
hf	-831.50	kJ/mol	Joback Method
hfus	38.63	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.049		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
tb	889.87	K	Joback Method
tc	1099.10	K	Joback Method
tf	582.81	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.81	J/mol×K	889.87	Joback Method
cpg	710.41	J/mol×K	924.74	Joback Method
cpg	720.00	J/mol×K	959.61	Joback Method
cpg	728.61	J/mol×K	994.49	Joback Method
cpg	736.25	J/mol×K	1029.36	Joback Method
cpg	742.93	J/mol×K	1064.23	Joback Method
cpg	748.66	J/mol×K	1099.10	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=C55712680&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume