Acetamide, n-(beta,3,4-trihydroxyphenethyl)-, 3,4-diacetate

Inchi: InChI=1S/C14H17NO6/c1-8(16)15-7-12(19)11-4-5-13(20-9(2)17)14(6-11)21-10(3)18/h4-
InchiKey: SBCYFIYIVXKFBL-UHFFFAOYSA-N
Formula: C14H17NO6
SMILES: CC(=O)NCC(O)c1ccc(OC(C)=O)c(OC(C)=O)c1
Mol. weight [g/mol]: 295.29
CAS: 109038-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-486.48	kJ/mol	Joback Method
hf	-824.92	kJ/mol	Joback Method
hfus	38.12	kJ/mol	Joback Method
hvap	98.14	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	0.707		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	904.72	K	Joback Method
tc	1117.80	K	Joback Method
tf	591.73	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.90	J/mol×K	904.72	Joback Method
cpg	663.41	J/mol×K	940.23	Joback Method
cpg	671.92	J/mol×K	975.75	Joback Method
cpg	679.42	J/mol×K	1011.26	Joback Method
cpg	685.93	J/mol×K	1046.77	Joback Method
cpg	691.44	J/mol×K	1082.29	Joback Method
cpg	695.96	J/mol×K	1117.80	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=C109038677&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume