Acetamide, N-[2-(acetyloxy)-2-[4-(acetyloxy)phenyl]ethyl]-

Other names: 4-(2-Aetylamino-1-(acetyloxy)ethyl)phenyl acetate
Inchi: InChI=1S/C14H17NO5/c1-9(16)15-8-14(20-11(3)18)12-4-6-13(7-5-12)19-10(2)17/h4-7,14
InchiKey: WELBTOLUOPVPJV-UHFFFAOYSA-N
Formula: C14H17NO5
SMILES: CC(=O)NCC(OC(C)=O)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 279.29
CAS: 55044-38-7

Physical Properties

Property code	Value	Unit	Source
gf	-340.03	kJ/mol	Joback Method
hf	-661.22	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.352		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	807.56	K	Joback Method
tc	1023.37	K	Joback Method
tf	518.39	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.75	J/mol×K	807.56	Joback Method
cpg	620.04	J/mol×K	843.53	Joback Method
cpg	631.29	J/mol×K	879.50	Joback Method
cpg	641.51	J/mol×K	915.47	Joback Method
cpg	650.71	J/mol×K	951.43	Joback Method
cpg	658.89	J/mol×K	987.40	Joback Method
cpg	666.07	J/mol×K	1023.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55044387&Units=SI
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

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