(2-acetamido-2-oxoethyl) benzoate

Inchi: InChI=1S/C11H11NO4/c1-8(13)12-10(14)7-16-11(15)9-5-3-2-4-6-9/h2-6H,7H2,1H3,(H,12
InchiKey: NZDAAPUTURAWII-UHFFFAOYSA-N
Formula: C11H11NO4
SMILES: CC(=O)NC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 221.21

Physical Properties

Property code	Value	Unit	Source
gf	-248.22	kJ/mol	Joback Method
hf	-450.33	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	71.44	kJ/mol	Joback Method
log10ws	-2.40		Aqueous Solubility Prediction Method
logp	0.506		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	711.96	K	Joback Method
tc	934.21	K	Joback Method
tf	377.65	K	Aqueous Solubility Prediction Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.97	J/mol×K	711.96	Joback Method
cpg	436.27	J/mol×K	749.00	Joback Method
cpg	446.69	J/mol×K	786.04	Joback Method
cpg	456.25	J/mol×K	823.09	Joback Method
cpg	464.97	J/mol×K	860.13	Joback Method
cpg	472.88	J/mol×K	897.17	Joback Method
cpg	480.00	J/mol×K	934.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume