(2-amino-2-oxoethyl) benzoate

Inchi: InChI=1S/C9H9NO3/c10-8(11)6-13-9(12)7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,11)
InchiKey: HBEWADIWKZVJSD-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: NC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 179.18

Physical Properties

Property code	Value	Unit	Source
gf	-159.08	kJ/mol	Joback Method
hf	-316.15	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-1.64		Aqueous Solubility Prediction Method
logp	0.329		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	634.69	K	Joback Method
tc	867.05	K	Joback Method
tf	422.96	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.45	J/mol×K	634.69	Joback Method
cpg	334.53	J/mol×K	673.42	Joback Method
cpg	344.80	J/mol×K	712.14	Joback Method
cpg	354.28	J/mol×K	750.87	Joback Method
cpg	362.98	J/mol×K	789.60	Joback Method
cpg	370.93	J/mol×K	828.33	Joback Method
cpg	378.14	J/mol×K	867.05	Joback Method

Sources

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
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