[2-[(2-amino-2-oxoethyl)-methylamino]-2-oxoethyl benzoate

Inchi: InChI=1S/C12H14N2O4/c1-14(7-10(13)15)11(16)8-18-12(17)9-5-3-2-4-6-9/h2-6H,7-8H2,

InchiKey: DLVAUVPZQHGFJC-UHFFFAOYSA-N

Formula: C12H14N2O4

SMILES: CN(CC(N)=O)C(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
gf	-151.96	kJ/mol	Joback Method
hf	-423.12	kJ/mol	Joback Method
hfus	35.08	kJ/mol	Joback Method
hvap	79.91	kJ/mol	Joback Method
log10ws	-0.92		Aqueous Solubility Prediction Method
logp	-0.213		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	769.64	K	Joback Method
tc	992.48	K	Joback Method
tf	374.65	K	Aqueous Solubility Prediction Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.61	J/mol×K	769.64	Joback Method
cpg	534.15	J/mol×K	806.78	Joback Method
cpg	544.72	J/mol×K	843.92	Joback Method
cpg	554.37	J/mol×K	881.06	Joback Method
cpg	563.12	J/mol×K	918.20	Joback Method
cpg	571.02	J/mol×K	955.34	Joback Method
cpg	578.11	J/mol×K	992.48	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