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

Inchi: InChI=1S/C12H15NO4/c1-13(7-8-14)11(15)9-17-12(16)10-5-3-2-4-6-10/h2-6,14H,7-9H2,

InchiKey: WRKNTBMMMVTKKA-UHFFFAOYSA-N

Formula: C12H15NO4

SMILES: CN(CCO)C(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 237.26

Physical Properties

Property code	Value	Unit	Source
gf	-226.31	kJ/mol	Joback Method
hf	-496.56	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-1.09		Aqueous Solubility Prediction Method
logp	0.294		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	735.42	K	Joback Method
tc	934.44	K	Joback Method
tf	466.80	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.65	J/mol×K	735.42	Joback Method
cpg	513.98	J/mol×K	768.59	Joback Method
cpg	524.55	J/mol×K	801.76	Joback Method
cpg	534.36	J/mol×K	834.93	Joback Method
cpg	543.46	J/mol×K	868.10	Joback Method
cpg	551.88	J/mol×K	901.27	Joback Method
cpg	559.63	J/mol×K	934.44	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