[2-(ethyl-(2-hydroxyethyl)amino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C13H17NO4/c1-2-14(8-9-15)12(16)10-18-13(17)11-6-4-3-5-7-11/h3-7,15H,2,8-

InchiKey: IIZIPXWXNPFUOU-UHFFFAOYSA-N

Formula: C13H17NO4

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

Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	-217.89	kJ/mol	Joback Method
hf	-517.20	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-1.37		Aqueous Solubility Prediction Method
logp	0.684		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	758.30	K	Joback Method
tc	956.02	K	Joback Method
tf	478.07	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.59	J/mol×K	758.30	Joback Method
cpg	567.38	J/mol×K	791.25	Joback Method
cpg	578.37	J/mol×K	824.21	Joback Method
cpg	588.59	J/mol×K	857.16	Joback Method
cpg	598.07	J/mol×K	890.11	Joback Method
cpg	606.84	J/mol×K	923.07	Joback Method
cpg	614.93	J/mol×K	956.02	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