[2-(bis(2-methoxyethyl)amino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C15H21NO5/c1-19-10-8-16(9-11-20-2)14(17)12-21-15(18)13-6-4-3-5-7-13/h3-

InchiKey: LJCFRMUKLSCNKV-UHFFFAOYSA-N

Formula: C15H21NO5

SMILES: COCCN(CCOC)C(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 295.33

Physical Properties

Property code	Value	Unit	Source
gf	-274.23	kJ/mol	Joback Method
hf	-670.69	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-1.57		Aqueous Solubility Prediction Method
logp	0.965		Crippen Method
mcvol	229.180	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
tb	756.72	K	Joback Method
tc	956.88	K	Joback Method
tf	330.65	K	Aqueous Solubility Prediction Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.11	J/mol×K	756.72	Joback Method
cpg	676.76	J/mol×K	790.08	Joback Method
cpg	690.39	J/mol×K	823.44	Joback Method
cpg	703.04	J/mol×K	856.80	Joback Method
cpg	714.69	J/mol×K	890.16	Joback Method
cpg	725.37	J/mol×K	923.52	Joback Method
cpg	735.09	J/mol×K	956.88	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