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

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

InchiKey: LDCFNNYCIXKMNJ-UHFFFAOYSA-N

Formula: C15H21NO5

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

Mol. weight [g/mol]: 295.33

Physical Properties

Property code	Value	Unit	Source
gf	-342.75	kJ/mol	Joback Method
hf	-721.27	kJ/mol	Joback Method
hfus	37.18	kJ/mol	Joback Method
hvap	101.79	kJ/mol	Joback Method
log10ws	-1.18		Aqueous Solubility Prediction Method
logp	0.434		Crippen Method
mcvol	229.180	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	895.36	K	Joback Method
tc	1099.76	K	Joback Method
tf	378.65	K	Aqueous Solubility Prediction Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.44	J/mol×K	895.36	Joback Method
cpg	728.14	J/mol×K	929.43	Joback Method
cpg	737.99	J/mol×K	963.49	Joback Method
cpg	747.03	J/mol×K	997.56	Joback Method
cpg	755.32	J/mol×K	1031.62	Joback Method
cpg	762.89	J/mol×K	1065.69	Joback Method
cpg	769.77	J/mol×K	1099.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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