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

Inchi: InChI=1S/C13H17NO5/c15-8-6-14(7-9-16)12(17)10-19-13(18)11-4-2-1-3-5-11/h1-5,15-16

InchiKey: UCIUVGVKELKZSD-UHFFFAOYSA-N

Formula: C13H17NO5

SMILES: O=C(OCC(=O)N(CCO)CCO)c1ccccc1

Mol. weight [g/mol]: 267.28

Physical Properties

Property code	Value	Unit	Source
gf	-354.71	kJ/mol	Joback Method
hf	-669.43	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	0.43		Aqueous Solubility Prediction Method
logp	-0.343		Crippen Method
mcvol	201.000	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	850.48	K	Joback Method
tc	1048.41	K	Joback Method
tf	538.89	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.81	J/mol×K	850.48	Joback Method
cpg	614.55	J/mol×K	883.47	Joback Method
cpg	623.57	J/mol×K	916.46	Joback Method
cpg	631.90	J/mol×K	949.44	Joback Method
cpg	639.57	J/mol×K	982.43	Joback Method
cpg	646.61	J/mol×K	1015.42	Joback Method
cpg	653.05	J/mol×K	1048.41	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