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

Inchi: InChI=1S/C17H25NO3/c1-13(2)10-18(11-14(3)4)16(19)12-21-17(20)15-8-6-5-7-9-15/h5-9

InchiKey: KXYFWLVSYHRZJL-UHFFFAOYSA-N

Formula: C17H25NO3

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

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-52.27	kJ/mol	Joback Method
hf	-458.09	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-3.56		Aqueous Solubility Prediction Method
logp	2.984		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	756.76	K	Joback Method
tc	961.14	K	Joback Method
tf	317.65	K	Aqueous Solubility Prediction Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.62	J/mol×K	756.76	Joback Method
cpg	735.07	J/mol×K	790.82	Joback Method
cpg	750.41	J/mol×K	824.89	Joback Method
cpg	764.70	J/mol×K	858.95	Joback Method
cpg	777.96	J/mol×K	893.01	Joback Method
cpg	790.26	J/mol×K	927.07	Joback Method
cpg	801.62	J/mol×K	961.14	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