[2-[(2-ethoxy-2-oxoethyl)-methylamino]-2-oxoethy benzoate

Inchi: InChI=1S/C14H17NO5/c1-3-19-13(17)9-15(2)12(16)10-20-14(18)11-7-5-4-6-8-11/h4-8H,

InchiKey: VPGYQOPHCDIWSQ-UHFFFAOYSA-N

Formula: C14H17NO5

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

Mol. weight [g/mol]: 279.29

Physical Properties

Property code	Value	Unit	Source
gf	-306.57	kJ/mol	Joback Method
hf	-630.41	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-1.67		Aqueous Solubility Prediction Method
logp	0.865		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	765.29	K	Joback Method
tc	974.65	K	Joback Method
tf	312.65	K	Aqueous Solubility Prediction Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.95	J/mol×K	765.29	Joback Method
cpg	608.99	J/mol×K	800.18	Joback Method
cpg	621.04	J/mol×K	835.08	Joback Method
cpg	632.11	J/mol×K	869.97	Joback Method
cpg	642.23	J/mol×K	904.86	Joback Method
cpg	651.42	J/mol×K	939.76	Joback Method
cpg	659.70	J/mol×K	974.65	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