[2-[(1-amino-1-oxopropan-2-yl)amino]-2-oxoethyl] benzoate

Inchi: InChI=1S/C12H14N2O4/c1-8(11(13)16)14-10(15)7-18-12(17)9-5-3-2-4-6-9/h2-6,8H,7H2,

InchiKey: GUNGCOIXSOZDCM-UHFFFAOYSA-N

Formula: C12H14N2O4

SMILES: CC(NC(=O)COC(=O)c1ccccc1)C(N)=O

Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
gf	-175.79	kJ/mol	Joback Method
hf	-442.46	kJ/mol	Joback Method
hfus	33.63	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-2.72		Aqueous Solubility Prediction Method
logp	-0.167		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	806.93	K	Joback Method
tc	1035.22	K	Joback Method
tf	474.65	K	Aqueous Solubility Prediction Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.46	J/mol×K	806.93	Joback Method
cpg	544.37	J/mol×K	844.98	Joback Method
cpg	554.28	J/mol×K	883.03	Joback Method
cpg	563.23	J/mol×K	921.07	Joback Method
cpg	571.24	J/mol×K	959.12	Joback Method
cpg	578.36	J/mol×K	997.17	Joback Method
cpg	584.60	J/mol×K	1035.22	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