Benzoic acid, p-[(3-amino-2-oxopropyl)amino]-, ethyl ester, oxime

Inchi: InChI=1S/C12H17N3O3/c1-2-18-12(16)9-3-5-10(6-4-9)14-8-11(7-13)15-17/h3-6,14,17H,2

InchiKey: RXTNMLUPCVQUKL-RVDMUPIBSA-N

Formula: C12H17N3O3

SMILES: CCOC(=O)c1ccc(NCC(CN)=NO)cc1

Mol. weight [g/mol]: 251.28

CAS: 23852-97-3

Physical Properties

Property code	Value	Unit	Source
hf	-303.29	kJ/mol	Joback Method
hvap	91.55	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.064		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	873.35	K	Joback Method
tc	1091.96	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23852973&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

hf: Enthalpy of formation 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