(2-ethylamino-2-oxoethyl) benzoate

Inchi: InChI=1S/C11H13NO3/c1-2-12-10(13)8-15-11(14)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,12,
InchiKey: FPWKJKWOCSENMO-UHFFFAOYSA-N
Formula: C11H13NO3
SMILES: CCNC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 207.23

Physical Properties

Property code	Value	Unit	Source
gf	-119.30	kJ/mol	Joback Method
hf	-337.75	kJ/mol	Joback Method
hfus	27.77	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-2.24		Aqueous Solubility Prediction Method
logp	0.979		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	658.09	K	Joback Method
tc	874.19	K	Joback Method
tf	414.90	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.45	J/mol×K	658.09	Joback Method
cpg	425.29	J/mol×K	694.11	Joback Method
cpg	437.25	J/mol×K	730.12	Joback Method
cpg	448.38	J/mol×K	766.14	Joback Method
cpg	458.69	J/mol×K	802.16	Joback Method
cpg	468.20	J/mol×K	838.18	Joback Method
cpg	476.94	J/mol×K	874.19	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