(2-methylamino-2-oxoethyl) benzoate

Inchi: InChI=1S/C10H11NO3/c1-11-9(12)7-14-10(13)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,11,12)
InchiKey: ZWAHHEQQTJUTPW-UHFFFAOYSA-N
Formula: C10H11NO3
SMILES: CNC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
gf	-127.72	kJ/mol	Joback Method
hf	-317.11	kJ/mol	Joback Method
hfus	25.18	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-1.72		Aqueous Solubility Prediction Method
logp	0.589		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	635.21	K	Joback Method
tc	855.07	K	Joback Method
tf	384.65	K	Aqueous Solubility Prediction Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.30	J/mol×K	635.21	Joback Method
cpg	375.49	J/mol×K	671.85	Joback Method
cpg	386.85	J/mol×K	708.50	Joback Method
cpg	397.40	J/mol×K	745.14	Joback Method
cpg	407.16	J/mol×K	781.78	Joback Method
cpg	416.15	J/mol×K	818.42	Joback Method
cpg	424.40	J/mol×K	855.07	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