(2-dimethylamino-2-oxoethyl) benzoate

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

Physical Properties

Property code	Value	Unit	Source
gf	-97.91	kJ/mol	Joback Method
hf	-323.69	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-1.37		Aqueous Solubility Prediction Method
logp	0.932		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	620.36	K	Joback Method
tc	834.16	K	Joback Method
tf	354.65	K	Aqueous Solubility Prediction Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.97	J/mol×K	620.36	Joback Method
cpg	413.56	J/mol×K	655.99	Joback Method
cpg	426.24	J/mol×K	691.63	Joback Method
cpg	438.06	J/mol×K	727.26	Joback Method
cpg	449.03	J/mol×K	762.90	Joback Method
cpg	459.20	J/mol×K	798.53	Joback Method
cpg	468.58	J/mol×K	834.16	Joback Method

Sources

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

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