[2-(acetyl-methylamino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C12H13NO4/c1-9(14)13(2)11(15)8-17-12(16)10-6-4-3-5-7-10/h3-7H,8H2,1-2H
InchiKey: JQUIGGQYRQVIIE-UHFFFAOYSA-N
Formula: C12H13NO4
SMILES: CC(=O)N(C)C(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 235.24

Physical Properties

Property code	Value	Unit	Source
gf	-218.41	kJ/mol	Joback Method
hf	-456.91	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-0.49		Aqueous Solubility Prediction Method
logp	0.848		Crippen Method
mcvol	176.740	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	697.11	K	Joback Method
tc	913.89	K	Joback Method
tf	375.65	K	Aqueous Solubility Prediction Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.89	J/mol×K	697.11	Joback Method
cpg	477.47	J/mol×K	733.24	Joback Method
cpg	489.11	J/mol×K	769.37	Joback Method
cpg	499.84	J/mol×K	805.50	Joback Method
cpg	509.71	J/mol×K	841.63	Joback Method
cpg	518.74	J/mol×K	877.76	Joback Method
cpg	526.96	J/mol×K	913.89	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