[2-oxo-2-(propan-2-ylamino)ethyl] benzoate

Inchi: InChI=1S/C12H15NO3/c1-9(2)13-11(14)8-16-12(15)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3,

InchiKey: FUWATACATASMHP-UHFFFAOYSA-N

Formula: C12H15NO3

SMILES: CC(C)NC(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 221.26

Physical Properties

Property code	Value	Unit	Source
gf	-113.32	kJ/mol	Joback Method
hf	-363.67	kJ/mol	Joback Method
hfus	26.84	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-2.73		Aqueous Solubility Prediction Method
logp	1.368		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	680.53	K	Joback Method
tc	897.17	K	Joback Method
tf	402.65	K	Aqueous Solubility Prediction Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.56	J/mol×K	680.53	Joback Method
cpg	477.22	J/mol×K	716.64	Joback Method
cpg	489.94	J/mol×K	752.74	Joback Method
cpg	501.74	J/mol×K	788.85	Joback Method
cpg	512.66	J/mol×K	824.95	Joback Method
cpg	522.72	J/mol×K	861.06	Joback Method
cpg	531.94	J/mol×K	897.17	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