[2-(di(propan-2-yl)amino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C15H21NO3/c1-11(2)16(12(3)4)14(17)10-19-15(18)13-8-6-5-7-9-13/h5-9,11-12
InchiKey: ZWUAUTPCFIIFAS-UHFFFAOYSA-N
Formula: C15H21NO3
SMILES: CC(C)N(C(=O)COC(=O)c1ccccc1)C(C)C
Mol. weight [g/mol]: 263.34

Physical Properties

Property code	Value	Unit	Source
gf	-69.11	kJ/mol	Joback Method
hf	-416.81	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-3.34		Aqueous Solubility Prediction Method
logp	2.489		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
tb	711.00	K	Joback Method
tc	919.84	K	Joback Method
tf	378.65	K	Aqueous Solubility Prediction Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.88	J/mol×K	711.00	Joback Method
cpg	623.84	J/mol×K	745.81	Joback Method
cpg	638.73	J/mol×K	780.61	Joback Method
cpg	652.58	J/mol×K	815.42	Joback Method
cpg	665.44	J/mol×K	850.23	Joback Method
cpg	677.33	J/mol×K	885.04	Joback Method
cpg	688.31	J/mol×K	919.84	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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

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