[2-(tert-butylamino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C13H17NO3/c1-13(2,3)14-11(15)9-17-12(16)10-7-5-4-6-8-10/h4-8H,9H2,1-3H
InchiKey: NZNPHIKNHGRVLZ-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: CC(C)(C)NC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-99.62	kJ/mol	Joback Method
hf	-387.78	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	67.85	kJ/mol	Joback Method
log10ws	-2.87		Aqueous Solubility Prediction Method
logp	1.758		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
tb	700.62	K	Joback Method
tc	921.10	K	Joback Method
tf	385.65	K	Aqueous Solubility Prediction Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.68	J/mol×K	700.62	Joback Method
cpg	531.96	J/mol×K	737.37	Joback Method
cpg	545.18	J/mol×K	774.11	Joback Method
cpg	557.40	J/mol×K	810.86	Joback Method
cpg	568.66	J/mol×K	847.60	Joback Method
cpg	579.03	J/mol×K	884.35	Joback Method
cpg	588.55	J/mol×K	921.10	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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