(2-diethylamino-2-oxoethyl) benzoate

Inchi: InChI=1S/C13H17NO3/c1-3-14(4-2)12(15)10-17-13(16)11-8-6-5-7-9-11/h5-9H,3-4,10H2,
InchiKey: MTAAHMQCSJMGHI-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: CCN(CC)C(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-81.07	kJ/mol	Joback Method
hf	-364.97	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-2.07		Aqueous Solubility Prediction Method
logp	1.712		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	666.12	K	Joback Method
tc	873.37	K	Joback Method
tf	345.65	K	Aqueous Solubility Prediction Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.75	J/mol×K	666.12	Joback Method
cpg	515.40	J/mol×K	700.66	Joback Method
cpg	529.09	J/mol×K	735.20	Joback Method
cpg	541.87	J/mol×K	769.74	Joback Method
cpg	553.76	J/mol×K	804.28	Joback Method
cpg	564.81	J/mol×K	838.83	Joback Method
cpg	575.03	J/mol×K	873.37	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