[2-(di(prop-2-enyl)amino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C15H17NO3/c1-3-10-16(11-4-2)14(17)12-19-15(18)13-8-6-5-7-9-13/h3-9H,1-2
InchiKey: KIBXYDHXHWRNTP-UHFFFAOYSA-N
Formula: C15H17NO3
SMILES: C=CCN(CC=C)C(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 259.31

Physical Properties

Property code	Value	Unit	Source
gf	111.45	kJ/mol	Joback Method
hf	-155.39	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-2.56		Aqueous Solubility Prediction Method
logp	2.044		Crippen Method
mcvol	208.840	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
tb	705.24	K	Joback Method
tc	913.89	K	Joback Method
tf	315.65	K	Aqueous Solubility Prediction Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.89	J/mol×K	705.24	Joback Method
cpg	573.18	J/mol×K	740.01	Joback Method
cpg	586.50	J/mol×K	774.79	Joback Method
cpg	598.88	J/mol×K	809.56	Joback Method
cpg	610.37	J/mol×K	844.34	Joback Method
cpg	621.02	J/mol×K	879.11	Joback Method
cpg	630.88	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