(2-oxo-2-propylaminoethyl) benzoate

Inchi: InChI=1S/C12H15NO3/c1-2-8-13-11(14)9-16-12(15)10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,
InchiKey: OLCZSUFMDPGDIL-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: CCCNC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 221.26

Physical Properties

Property code	Value	Unit	Source
gf	-110.88	kJ/mol	Joback Method
hf	-358.39	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	66.92	kJ/mol	Joback Method
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	1.370		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	680.97	K	Joback Method
tc	893.66	K	Joback Method
tf	362.65	K	Aqueous Solubility Prediction Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.02	J/mol×K	680.97	Joback Method
cpg	476.41	J/mol×K	716.42	Joback Method
cpg	488.89	J/mol×K	751.87	Joback Method
cpg	500.51	J/mol×K	787.31	Joback Method
cpg	511.28	J/mol×K	822.76	Joback Method
cpg	521.23	J/mol×K	858.21	Joback Method
cpg	530.38	J/mol×K	893.66	Joback Method

Sources

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

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