[2-(cyclohexylamino)-2-oxoethyl] benzoate

Inchi: InChI=1S/C15H19NO3/c17-14(16-13-9-5-2-6-10-13)11-19-15(18)12-7-3-1-4-8-12/h1,3-4,

InchiKey: DQMPCJPRPFRUIT-UHFFFAOYSA-N

Formula: C15H19NO3

SMILES: O=C(COC(=O)c1ccccc1)NC1CCCCC1

Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
gf	-61.17	kJ/mol	Joback Method
hf	-365.99	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-3.90		Aqueous Solubility Prediction Method
logp	2.292		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	769.16	K	Joback Method
tc	1003.18	K	Joback Method
tf	467.36	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.59	J/mol×K	769.16	Joback Method
cpg	632.02	J/mol×K	808.16	Joback Method
cpg	647.03	J/mol×K	847.17	Joback Method
cpg	660.68	J/mol×K	886.17	Joback Method
cpg	673.01	J/mol×K	925.18	Joback Method
cpg	684.08	J/mol×K	964.18	Joback Method
cpg	693.93	J/mol×K	1003.18	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