4-(4-Chlorobenzoyl)morpholine

Other names: 4-Chlorobenzoic acid, morpholide
Inchi: InChI=1S/C11H12ClNO2/c12-10-3-1-9(2-4-10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2
InchiKey: BGRFQNTYHMHVFJ-UHFFFAOYSA-N
Formula: C11H12ClNO2
SMILES: O=C(c1ccc(Cl)cc1)N1CCOCC1
Mol. weight [g/mol]: 225.68

Physical Properties

Property code	Value	Unit	Source
hf	-241.20	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-1.82		Cheméo Relay (1.0)
logp	1.812		Crippen Method
mcvol	160.890	ml/mol	McGowan Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	618.54	K	Cheméo Relay (1.0)
tf	335.72	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19202041&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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