

4-(4-Chlorobenzoyl)morpholine

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]:	225.67
CAS:	19202-04-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.812		Crippen Method
mcvol	160.890	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19202041&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/116-133-5/4-4-Chlorobenzoyl-morpholine.pdf>

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