

Morpholine, 4-(4-chloro-2-nitrophenyl)-

Other names: 4-(4-Chloro-2-nitrophenyl)morpholine
Inchi: InChI=1S/C10H11ClN2O3/c11-8-1-2-9(10(7-8)13(14)15)12-3-5-16-6-4-12/h1-2,7H,3-6H2
InchiKey: KJISHWYSNGQNFM-UHFFFAOYSA-N
Formula: C10H11ClN2O3
SMILES: O=[N+]([O-])c1cc(Cl)ccc1N1CCOCC1
Mol. weight [g/mol]: 242.66
CAS: 65976-60-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	2.085		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
rinpol	1857.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65976605&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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