1-(3,4-dichlorophenyl)piperazine

Inchi: InChI=1S/C10H12Cl2N2/c11-9-2-1-8(7-10(9)12)14-5-3-13-4-6-14/h1-2,7,13H,3-6H2
InchiKey: PXFJLKKZSWWVRX-UHFFFAOYSA-N
Formula: C10H12Cl2N2
SMILES: Clc1ccc(N2CCNCC2)cc1Cl
Mol. weight [g/mol]: 231.12
CAS: 57260-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	2.403		Crippen Method
mcvol	161.580	ml/mol	McGowan Method

Sources

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=C57260670&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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