

# 1-(3,4-dichlorophenyl)piperazine

<b>Inchi:</b>	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
<b>InchiKey:</b>	PXFJLKKZSWWVRX-UHFFFAOYSA-N
<b>Formula:</b>	C10H12Cl2N2
<b>SMILES:</b>	Clc1ccc(N2CCNCC2)cc1Cl
<b>Mol. weight [g/mol]:</b>	231.12
<b>CAS:</b>	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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57260670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57260670&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/122-209-4/1-3-4-dichlorophenyl-piperazine.pdf>

Generated by Cheméo on 2024-04-29 08:48:45.207975148 +0000 UTC m=+16669774.128552459.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.