

Pyrazine, 2-chloro-3-(4-methylphenyl)-

Inchi:	InChI=1S/C11H9ClN2/c1-8-2-4-9(5-3-8)10-11(12)14-7-6-13-10/h2-7H,1H3
InchiKey:	UNLHAQUSIBUXFE-UHFFFAOYSA-N
Formula:	C11H9ClN2
SMILES:	Cc1ccc(-c2nccnc2Cl)cc1
Mol. weight [g/mol]:	204.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.105		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380557&Units=SI
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

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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<https://www.chemeo.com/cid/115-509-9/Pyrazine-2-chloro-3-4-methylphenyl.pdf>

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