

2-(P-chlorophenyl mercapto)-3-methyl pyrazine

Inchi:	InChI=1S/C11H9ClN2S/c1-8-11(14-7-6-13-8)15-10-4-2-9(12)3-5-10/h2-7H,1H3
InchiKey:	VWHRCENLDVGZPJ-UHFFFAOYSA-N
Formula:	C11H9ClN2S
SMILES:	<chem>Cc1nccnc1Sc1ccc(Cl)cc1</chem>
Mol. weight [g/mol]:	236.72
CAS:	116660-15-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	3.590		Crippen Method
mcvol	166.880	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=C116660152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/118-963-2/2-P-chlorophenyl-mercapto-3-methyl-pyrazine.pdf>

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