

3-Methyl-4-phenylpyrazole

Inchi:	InChI=1S/C10H10N2/c1-8-10(7-11-12-8)9-5-3-2-4-6-9/h2-7H,1H3,(H,11,12)
InchiKey:	XTXZCNATVCIKTR-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Cc1n[nH]cc1-c1ccccc1
Mol. weight [g/mol]:	158.20
CAS:	13788-84-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.903		Crippen Method
mcvol	128.500	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13788846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/55-588-9/3-Methyl-4-phenylpyrazole.pdf>

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