

1,3,5-Trimethyl-1H-pyrazol-4-amine

Other names:	4-Amino-1,3,5-trimethylpyrazole
Inchi:	InChI=1S/C6H11N3/c1-4-6(7)5(2)9(3)8-4/h7H2,1-3H3
InchiKey:	SSDGMKHZMNTWLS-UHFFFAOYSA-N
Formula:	C6H11N3
SMILES:	Cc1nn(C)c(C)c1N
Mol. weight [g/mol]:	125.17
CAS:	28466-21-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	0.619		Crippen Method
mcvol	105.880	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=C28466219&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/17-544-9/1-3-5-Trimethyl-1H-pyrazol-4-amine.pdf>

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