

Pyrazole, 4-nitro-1,3,5-trimethyl-

Other names:	4-Nitro-1,3,5-trimethylpyrazole
Inchi:	InChI=1S/C6H9N3O2/c1-4-6(9(10)11)5(2)8(3)7-4/h1-3H3
InchiKey:	YSZYFGMARJFMJK-UHFFFAOYSA-N
Formula:	C6H9N3O2
SMILES:	<chem>Cc1nn(C)c(C)c1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	155.15
CAS:	1125-30-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	0.945		Crippen Method
mcvol	113.320	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=C1125300&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

Latest version available from:

<https://www.chemeo.com/cid/34-639-5/Pyrazole-4-nitro-1-3-5-trimethyl.pdf>

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