

1H-PYRAZOLE, 3,5-BIS(1,1-DIMETHYLETHYL)-

Other names:	3,5-di-t-Butylpyrazole
Inchi:	InChI=1S/C11H20N2/c1-10(2,3)8-7-9(13-12-8)11(4,5)6/h7H,1-6H3,(H,12,13)
InchiKey:	UEQDCVLVDQENIN-UHFFFAOYSA-N
Formula:	C11H20N2
SMILES:	CC(C)(C)c1cc(C(C)(C)C)[nH]n1
Mol. weight [g/mol]:	180.30

Physical Properties

Property code	Value	Unit	Source
affp	952.70	kJ/mol	NIST Webbook
basg	920.80	kJ/mol	NIST Webbook
logp	2.523		Crippen Method
mcvol	166.350	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1132145&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/81-572-7/1H-PYRAZOLE-3-5-BIS-1-1-DIMETHYLETHYL.pdf>

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