

N-t-Butylpyrrole

Other names:	1-tert-Butylpyrrole 1H-Pyrrole, 1-(1,1-dimethylethyl)-
Inchi:	InChI=1S/C8H13N/c1-8(2,3)9-6-4-5-7-9/h4-7H,1-3H3
InchiKey:	GJIRIQBRSTYPSF-UHFFFAOYSA-N
Formula:	C8H13N
SMILES:	CC(C)(C)n1cccc1
Mol. weight [g/mol]:	123.20
CAS:	24764-40-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	2.243		Crippen Method
mcvol	114.100	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C24764407&Units=SI

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/57-958-6/N-t-Butylpyrrole.pdf>

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