

4-Bromo-1,3,5-trimethylpyrazole

Inchi:	InChI=1S/C6H9BrN2/c1-4-6(7)5(2)9(3)8-4/h1-3H3
InchiKey:	UNTQXOJGXGRHMG-UHFFFAOYSA-N
Formula:	C6H9BrN2
SMILES:	Cc1nn(C)c(C)c1Br
Mol. weight [g/mol]:	189.05
CAS:	15801-69-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	1.799		Crippen Method
mcvol	113.400	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C15801691&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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