

1H-Imidazole, 2,4,5-tribromo-

Other names:	Imidazole, 2,4,5-tribromo- 2,4,5-Tribromoimidazole
Inchi:	InChI=1S/C3HBr3N2/c4-1-2(5)8-3(6)7-1/h(H,7,8)
InchiKey:	JCGGPCDDFXIVQB-UHFFFAOYSA-N
Formula:	C3HBr3N2
SMILES:	Brc1nc(Br)c(Br)[nH]1
Mol. weight [g/mol]:	304.76
CAS:	2034-22-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	2.215		Crippen Method
mcvol	106.130	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=C2034222&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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