

1H-1,2,4-Triazole, 3-bromo-5-methyl-

Other names:	s-Triazole, 3-bromo-5-methyl-
Inchi:	InChI=1S/C3H4BrN3/c1-2-5-3(4)7-6-2/h1H3,(H,5,6,7)
InchiKey:	BMTIGKUJWSEHHI-UHFFFAOYSA-N
Formula:	C3H4BrN3
SMILES:	Cc1nc(Br)n[nH]1
Mol. weight [g/mol]:	161.99
CAS:	26557-90-4

Physical Properties

Property code	Value	Unit	Source
ie	9.60	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	0.394		Crippen Method
mcvol	81.110	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26557904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
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/65-643-6/1H-1-2-4-Triazole-3-bromo-5-methyl.pdf>

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