3-Bromo-1H-1,2,4-triazole

Other names:	s-Triazole, 3-bromo-
	3-Bromo-1,2,4-triazole
	3-Bromo-1H-1,2,4-triazole
	1H-1,2,4-Triazole,5-bromo-
Inchi:	InChI=1S/C2H2BrN3/c3-2-4-1-5-6-2/h1H,(H,4,5,6)
InchiKey:	HHIZISRHAQPAMY-UHFFFAOYSA-N
Formula:	C2H2BrN3
SMILES:	Brc1nc[nH]n1
Mol. weight [g/mol]:	147.96

Physical Properties

Property code	Value	Unit	Source
ie	9.90	eV	NIST Webbook
log10ws	-0.42		Cheméo Relay (1.0)
logp	0.085		Crippen Method
mcvol	67.020	ml/mol	McGowan Method
tf	392.41	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7343331&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point