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