1H-Tetrazole, 5-vinyl-

Other names: 5-ethenyl-1H-tetrazole
Inchi: InChI=1S/C3H4N4/c1-2-3-4-6-7-5-3/h2H,1H2,(H,4,5,6,7)
InchiKey: VTQMJCSAHXYXPJ-UHFFFAOYSA-N
Formula: C3H4N4
SMILES: C=Cc1nn[nH]n1
Mol. weight [g/mol]: 96.09
CAS: 18755-47-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.81		Crippen Method
logp	-0.639		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

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=C18755470&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume