1H-1,2,4-Triazole, 3-propyl-

Other names: s-Triazole, 3-propyl-
Inchi: InChI=1S/C5H9N3/c1-2-3-5-6-4-7-8-5/h4H,2-3H2,1H3,(H,6,7,8)
InchiKey: ZFWJVKLPEZPKNL-UHFFFAOYSA-N
Formula: C5H9N3
SMILES: CCCc1nc[nH]n1
Mol. weight [g/mol]: 111.15
CAS: 19932-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	0.275		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	1172.00		NIST Webbook
rinpol	1172.00		NIST Webbook

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=C19932606&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
rinpol: Non-polar retention indices

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