

1H-1,2,4-Triazol-3-amine, 1-propyl-

Other names:	1H-1,2,4-Triazole-3-amine,1-propyl-
Inchi:	InChI=1S/C5H10N4/c1-2-3-9-4-7-5(6)8-9/h4H,2-3H2,1H3,(H2,6,8)
InchiKey:	RWJOWQPWDQMLRB-UHFFFAOYSA-N
Formula:	C5H10N4
SMILES:	CCCN1cnc(N)n1
Mol. weight [g/mol]:	126.16
CAS:	58661-95-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Crippen Method
logp	0.270		Crippen Method
mcvol	101.770	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58661953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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/70-241-6/1H-1-2-4-Triazol-3-amine-1-propyl.pdf>

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