

[1,2,4]Triazolo[1,5-a]pyridine

Other names:	s-Triazolo[1,5-a]pyridine 1,3-Diazaindolizine 1,3,3a-Triazaindene
Inchi:	InChI=1S/C6H5N3/c1-2-4-9-6(3-1)7-5-8-9/h1-5H
InchiKey:	DACWQSNZECJJGG-UHFFFAOYSA-N
Formula:	C6H5N3
SMILES:	c1ccn2ncnc2c1
Mol. weight [g/mol]:	119.12
CAS:	274-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	0.729		Crippen Method
mcvol	86.420	ml/mol	McGowan Method
ripol	1675.00		NIST Webbook
ripol	1675.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C274851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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