

S-Triazolo(1,5-a)pyrimidine, 5-methyl-7-ethylamino-

Other names:	(1,2,4)Triazolo(1,5-a)pyrimidin-7-amine, N-ethyl-5-methyl-5-Methyl-7-ethylamino-s-triazolo(1,5-a)pyrimidine 4-Ethylamino-6-methyl-1,3,3a,7-tetrazaindene
Inchi:	InChI=1S/C8H11N5/c1-3-9-7-4-6(2)12-8-10-5-11-13(7)8/h4-5,9H,3H2,1-2H3
InchiKey:	JDYRAZLWDUVBMX-UHFFFAOYSA-N
Formula:	C8H11N5
SMILES:	CCNc1cc(C)nc2ncnn12
Mol. weight [g/mol]:	177.21
CAS:	51806-90-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	0.865		Crippen Method
mcvol	134.560	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51806907&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

Latest version available from:

<https://www.chemeo.com/cid/69-036-6/S-Triazolo-1-5-a-pyrimidine-5-methyl-7-ethylamino.pdf>

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