

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

Physical Properties

Property code	Value	Unit	Source
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>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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