

Pyrimido[5,4-e]-as-triazine-5(6h)-thione

Inchi:	InChI=1S/C5H3N5S/c11-5-3-4(7-1-8-5)10-9-2-6-3/h1-2H,(H,7,8,10,11)
InchiKey:	NXUXQHDXUVCKEY-UHFFFAOYSA-N
Formula:	C5H3N5S
SMILES:	S=c1[nH]cnc2nncnc12
Mol. weight [g/mol]:	165.18
CAS:	21308-96-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	-0.005		Crippen Method
mcvol	104.340	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21308963&Units=SI

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/72-960-6/Pyrimido-5-4-e-as-triazine-5-6h-thione.pdf>

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