

4,6-Dimethyl-2-mercaptopyridine-3-carbonitrile

Other names:	Pyridine-3-carbonitrile, 1,2-dihydro-4,6-dimethyl-2-thio-
Inchi:	InChI=1S/C8H8N2S/c1-5-3-6(2)10-8(11)7(5)4-9/h3H,1-2H3,(H,10,11)
InchiKey:	CZRHEROEPICLRO-UHFFFAOYSA-N
Formula:	C8H8N2S
SMILES:	<chem>Cc1cc(C)c(C#N)c(S)n1</chem>
Mol. weight [g/mol]:	164.23
CAS:	54585-47-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	1.859		Crippen Method
mcvol	127.530	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54585476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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