

4-Thiouracil

Inchi:	InChI=1S/C4H4N2OS/c7-4-5-2-1-3(8)6-4/h1-2H,(H2,5,6,7,8)
InchiKey:	OVONXEQQWXGFJD-UHFFFAOYSA-N
Formula:	C4H4N2OS
SMILES:	Oc1nccc(S)n1
Mol. weight [g/mol]:	128.15
CAS:	591-28-6

Physical Properties

Property code	Value	Unit	Source
ea	1.05 ± 0.10	eV	NIST Webbook
log10ws	-1.06		Crippen Method
logp	0.471		Crippen Method
mcvol	85.640	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=C591286&Units=SI

Legend

ea:	Electron affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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