

4H-Thiopyran-4-one

Other names:	Thiopyran-4-one 1,4-Thiapyrone 4-Thiapyrone 4-Thiopyrone 4H-Thiopyran, 4-oxo-
Inchi:	InChI=1S/C5H4OS/c6-5-1-3-7-4-2-5/h1-4H
InchiKey:	VNXUJPCYZSNXDG-UHFFFAOYSA-N
Formula:	C5H4OS
SMILES:	O=c1ccsc1
Mol. weight [g/mol]:	112.15
CAS:	1003-41-4

Physical Properties

Property code	Value	Unit	Source
ie	8.97 ± 0.05	eV	NIST Webbook
log10ws	-0.65		Crippen Method
logp	1.108		Crippen Method
mcvol	79.770	ml/mol	McGowan Method

Sources

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=C1003414&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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