

3H-1,2-Dithiole-3-thione, 5-methyl-

Inchi: InChI=1S/C4H4S3/c1-3-2-4(5)7-6-3/h2H,1H3
InchiKey: LEPDMIYUICCABX-UHFFFAOYSA-N
Formula: C4H4S3
SMILES: Cc1cc(=S)ss1
Mol. weight [g/mol]: 148.27
CAS: 3354-40-3

Physical Properties

Property code	Value	Unit	Source
ie	8.25	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.848		Crippen Method
mcvol	96.810	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3354403&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.chemeo.com/cid/80-718-6/3H-1-2-Dithiole-3-thione-5-methyl.pdf>

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