

2,5-dimethyl-3-(methylthio)furan

Other names: Furan,2,5-dimethyl-3-(methylthiol)-
Inchi: InChI=1S/C7H10OS/c1-5-4-7(9-3)6(2)8-5/h4H,1-3H3
InchiKey: DWAOFMNMQUXUGG-UHFFFAOYSA-N
Formula: C7H10OS
SMILES: CSc1cc(C)oc1C
Mol. weight [g/mol]: 142.22
CAS: 63359-63-7

Physical Properties

Property code	Value	Unit	Source
ie	7.91 ± 0.05	eV	NIST Webbook
log10ws	-6.90		Crippen Method
logp	2.618		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
ripol	1440.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C63359637&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
ripol: Polar retention indices

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