

2,6-Dimethyl-4-thiopyrone

Other names:	2,6-Dimethylpyran-4-thione 4H-Pyran-4-thione, 2,6-dimethyl- NSC 75204
Inchi:	InChI=1S/C7H8OS/c1-5-3-7(9)4-6(2)8-5/h3-4H,1-2H3
InchiKey:	RZGQBLWMLLDDKL-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	<chem>Cc1cc(=S)cc(C)o1</chem>
Mol. weight [g/mol]:	140.20
CAS:	1004-37-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	2.626		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/92-794-9/2-6-Dimethyl-4-thiopyrone.pdf>

Generated by Cheméo on 2025-12-05 18:07:29.92943534 +0000 UTC m=+4706247.459476003.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.