

4-Methoxy-6-methyl-2-thiopyrone

Other names:	6-Methyl-4-methoxy-2H-pyran-2-thione
Inchi:	InChI=1S/C7H8O2S/c1-5-3-6(8-2)4-7(10)9-5/h3-4H,1-2H3
InchiKey:	PVBKLSUHIMQNMU-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	<chem>COc1cc(C)oc(=S)c1</chem>
Mol. weight [g/mol]:	156.20
CAS:	52911-98-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	2.326		Crippen Method
mccvol	113.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	130.50 ± 5.90	kJ/mol	408.50	NIST Webbook
hvapt	108.90	kJ/mol	408.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.org/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52911985&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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