

4H-PYRAN-4-THIONE, 2,6-DIMETHYL-

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:	Cc1cc(=S)cc(C)o1
Mol. weight [g/mol]:	140.21

Physical Properties

Property code	Value	Unit	Source
hvap	100.40	kJ/mol	Cheméo Relay (1.0)
ie	8.15	eV	Cheméo Relay (1.0)
logp	2.626		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	511.53	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004371&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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