

CARBONIMIDODITHIOIC ACID, METHYL-, DIMETHYL ESTER

Other names:	Dimethyl methyldithioimidocarbonate N-Methyl-dithiocarbonimidic acid dimethyl ester
Inchi:	InChI=1S/C4H9NS2/c1-5-4(6-2)7-3/h1-3H3
InchiKey:	YUYOKNUOMDVHTO-UHFFFAOYSA-N
Formula:	C4H9NS2
SMILES:	CN=C(SC)SC
Mol. weight [g/mol]:	135.26

Physical Properties

Property code	Value	Unit	Source
chl	-4055.00	kJ/mol	NIST Webbook
hfl	-3.00	kJ/mol	NIST Webbook
ie	8.47	eV	Cheméo Relay (1.0)
logp	1.698		Crippen Method
mcvol	105.600	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18805259&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
hfl:	Liquid phase enthalpy of formation at standard conditions
ie:	Ionization energy

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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