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