

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]:	135.25
CAS:	18805-25-9

Physical Properties

Property code	Value	Unit	Source
hf	30.28	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.698		Crippen Method
mcvol	105.600	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	505.04	K	Joback Method
tc	750.42	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18805259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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