

Ethyl dithiocarbimidoic acid dimethyl ester

Inchi: InChI=1S/C5H11NS2/c1-4-6-5(7-2)8-3/h4H2,1-3H3
InchiKey: XUVXWQRJUHSQQC-UHFFFAOYSA-N
Formula: C5H11NS2
SMILES: CCN=C(SC)SC
Mol. weight [g/mol]: 149.28
CAS: 116072-47-0

Physical Properties

Property code	Value	Unit	Source
chl	-4728.13	kJ/mol	NIST Webbook
hf	9.64	kJ/mol	Joback Method
hfl	-13.20	kJ/mol	NIST Webbook
hvap	43.75	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	2.088		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	527.92	K	Joback Method
tc	768.45	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=C116072470&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chl: Standard liquid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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