Methyl dithiocarbimidoic acid diethyl ester

Inchi: InChI=1S/C6H13NS2/c1-4-8-6(7-3)9-5-2/h4-5H2,1-3H3
InchiKey: FXHHZKMGSMMZEJ-UHFFFAOYSA-N
Formula: C6H13NS2
SMILES: CCSC(=NC)SCC
Mol. weight [g/mol]: 163.30
CAS: 75534-76-8

Physical Properties

Property code	Value	Unit	Source
hf	-11.00	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.478		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	550.80	K	Joback Method
tc	786.57	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75534768&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: 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