Pheny dithiocarbimidoic acid dimethyl ester

Inchi: InChI=1S/C9H11NS2/c1-11-9(12-2)10-8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: LTPWYSQGZKSLIW-UHFFFAOYSA-N
Formula: C9H11NS2
SMILES: CSC(=Nc1ccccc1)SC
Mol. weight [g/mol]: 197.32
CAS: 18805-23-7

Physical Properties

Property code	Value	Unit	Source
chs	-6462.20	kJ/mol	NIST Webbook
hf	163.61	kJ/mol	Joback Method
hfs	143.00	kJ/mol	NIST Webbook
hvap	54.93	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.400		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	646.12	K	Joback Method
tc	919.66	K	Joback Method

Sources

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=C18805237&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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