3-(Methylthio)phenyl isothiocyanate

Inchi: InChI=1S/C8H7NS2/c1-11-8-4-2-3-7(5-8)9-6-10/h2-5H,1H3
InchiKey: IHKAGFVCXPFGRP-UHFFFAOYSA-N
Formula: C8H7NS2
SMILES: CSc1cccc(N=C=S)c1
Mol. weight [g/mol]: 181.28
CAS: 51333-80-3

Physical Properties

Property code	Value	Unit	Source
hf	342.55	kJ/mol	Joback Method
hvap	53.60	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.143		Crippen Method
mcvol	133.900	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	628.83	K	Joback Method
tc	910.41	K	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51333803&Units=SI

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