2-Cyanophenyl isothiocyanate

Inchi: InChI=1S/C8H4N2S/c9-5-7-3-1-2-4-8(7)10-6-11/h1-4H
InchiKey: GDHYPPBFBJXNRE-UHFFFAOYSA-N
Formula: C8H4N2S
SMILES: N#Cc1ccccc1N=C=S
Mol. weight [g/mol]: 160.20
CAS: 81431-98-3

Physical Properties

Property code	Value	Unit	Source
hf	465.56	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.293		Crippen Method
mcvol	118.930	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	662.13	K	Joback Method
tc	936.65	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=C81431983&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