

p-Vinylphenyl isothiocyanate

Inchi:	InChI=1S/C9H7NS/c1-2-8-3-5-9(6-4-8)10-7-11/h2-6H,1H2
InchiKey:	VLYLPZIBVLBOLH-UHFFFAOYSA-N
Formula:	C9H7NS
SMILES:	C=Cc1ccc(N=C=S)cc1
Mol. weight [g/mol]:	161.22
CAS:	1520-20-3

Physical Properties

Property code	Value	Unit	Source
hf	405.47	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.064		Crippen Method
mcvol	127.340	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	579.61	K	Joback Method
tc	840.71	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1520203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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