

4-Methyl-2-nitrophenyl isothiocyanate

Inchi: InChI=1S/C8H6N2O2S/c1-6-2-3-7(9-5-13)8(4-6)10(11)12/h2-4H,1H3
InchiKey: CUQUTWSUXWDJKF-UHFFFAOYSA-N
Formula: C8H6N2O2S
SMILES: Cc1ccc(N=C=S)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 194.21
CAS: 17614-74-3

Physical Properties

Property code	Value	Unit	Source
hf	278.45	kJ/mol	Joback Method
hvap	64.03	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.638		Crippen Method
mcvol	134.970	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	716.87	K	Joback Method
tc	1000.95	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17614743&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

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