

4-Methoxy-2-nitrophenyl isothiocyanate

Inchi:	InChI=1S/C8H6N2O3S/c1-13-6-2-3-7(9-5-14)8(4-6)10(11)12/h2-4H,1H3
InchiKey:	YVARXELMRLSEEG-UHFFFAOYSA-N
Formula:	C8H6N2O3S
SMILES:	COc1ccc(N=C=S)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	210.21
CAS:	23165-60-8

Physical Properties

Property code	Value	Unit	Source
hf	146.23	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.338		Crippen Method
mcvol	140.840	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	739.29	K	Joback Method
tc	1017.51	K	Joback Method

Sources

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=C23165608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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