

3,4-Dimethoxyphenyl isothiocyanate

Inchi:	InChI=1S/C9H9NO2S/c1-11-8-4-3-7(10-6-13)5-9(8)12-2/h3-5H,1-2H3
InchiKey:	LHPZZVZPOZPDDDB-UHFFFAOYSA-N
Formula:	C9H9NO2S
SMILES:	COc1ccc(N=C=S)cc1OC
Mol. weight [g/mol]:	195.24
CAS:	33904-04-0

Physical Properties

Property code	Value	Unit	Source
hf	4.13	kJ/mol	Joback Method
hvap	54.49	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.438		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	632.75	K	Joback Method
tc	880.39	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33904040&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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