

5-Chloro-2,4-dimethoxyphenyl isothiocyanate

Inchi: InChI=1S/C9H8ClNO2S/c1-12-8-4-9(13-2)7(11-5-14)3-6(8)10/h3-4H,1-2H3
InchiKey: BXJOFCAXBGIDIR-UHFFFAOYSA-N
Formula: C9H8ClNO2S
SMILES: COc1cc(OC)c(N=C=S)cc1Cl
Mol. weight [g/mol]: 229.68
CAS: 40046-27-3

Physical Properties

Property code	Value	Unit	Source
hf	-23.08	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.091		Crippen Method
mvol	155.620	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	675.16	K	Joback Method
tc	926.36	K	Joback Method

Sources

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=C40046273&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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