

3,4,5-TRIMETHOXYPHENYL ISOTHIOCYANATE

Other names:	3,4,5-Trimethoxyphenyl isothiocyanate
Inchi:	InChI=1S/C10H11NO3S/c1-12-8-4-7(11-6-15)5-9(13-2)10(8)14-3/h4-5H,1-3H3
InchiKey:	AFWKAIYTSPWWCA-UHFFFAOYSA-N
Formula:	C10H11NO3S
SMILES:	COc1cc(N=C=S)cc(OC)c1OC
Mol. weight [g/mol]:	225.27

Physical Properties

Property code	Value	Unit	Source
logp	2.447		Crippen Method
mcvol	163.340	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35967249&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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