

3,4-Dimethoxybenzyl isothiocyanate

Inchi:	InChI=1S/C10H11NO2S/c1-12-9-4-3-8(6-11-7-14)5-10(9)13-2/h3-5H,6H2,1-2H3
InchiKey:	MTKPIGBIMQONMN-UHFFFAOYSA-N
Formula:	C10H11NO2S
SMILES:	COc1ccc(CN=C=S)cc1OC
Mol. weight [g/mol]:	209.26
CAS:	14596-50-0

Physical Properties

Property code	Value	Unit	Source
hf	-16.51	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.307		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	655.63	K	Joback Method
tc	897.88	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=C14596500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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