

2,5-Dimethoxyphenyl isothiocyanate

Inchi: InChI=1S/C9H9NO2S/c1-11-7-3-4-9(12-2)8(5-7)10-6-13/h3-5H,1-2H3
InchiKey: RADQLZMDTYWZKA-UHFFFAOYSA-N
Formula: C9H9NO2S
SMILES: COc1ccc(OC)c(N=C=S)c1
Mol. weight [g/mol]: 195.24
CAS: 40532-06-7

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
mvol	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

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=C40532067&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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