2,3-Dimethoxybenzyl isothiocyanate

Inchi: InChI=1S/C10H11NO2S/c1-12-9-5-3-4-8(6-11-7-14)10(9)13-2/h3-5H,6H2,1-2H3
InchiKey: HLXLDIINPAOCAT-UHFFFAOYSA-N
Formula: C10H11NO2S
SMILES: COc1cccc(CN=C=S)c1OC
Mol. weight [g/mol]: 209.26
CAS: 34964-55-1

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34964551&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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