3,4-Dimethoxyphenethyl isothiocyanate

Inchi: InChI=1S/C11H13NO2S/c1-13-10-4-3-9(5-6-12-8-15)7-11(10)14-2/h3-4,7H,5-6H2,1-2H3
InchiKey: GHYFLDWHIVKQLS-UHFFFAOYSA-N
Formula: C11H13NO2S
SMILES: COc1ccc(CCN=C=S)cc1OC
Mol. weight [g/mol]: 223.29
CAS: 21714-25-0

Physical Properties

Property code	Value	Unit	Source
hf	-37.15	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.349		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	678.51	K	Joback Method
tc	915.72	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21714250&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

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