(2-Methoxy-5-phenyl)phenylisothiocyanate

Inchi: InChI=1S/C14H11NOS/c1-16-14-8-7-12(9-13(14)15-10-17)11-5-3-2-4-6-11/h2-9H,1H3
InchiKey: TZRMLJYZKZTEFW-UHFFFAOYSA-N
Formula: C14H11NOS
SMILES: COc1ccc(-c2ccccc2)cc1N=C=S
Mol. weight [g/mol]: 241.31
CAS: 206761-68-4

Physical Properties

Property code	Value	Unit	Source
hf	269.68	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.096		Crippen Method
mcvol	184.200	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	751.41	K	Joback Method
tc	1024.56	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C206761684&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