2-(4-Methylphenylthio)phenyl isothiocyanate

Inchi: InChI=1S/C14H11NS2/c1-11-6-8-12(9-7-11)17-14-5-3-2-4-13(14)15-10-16/h2-9H,1H3
InchiKey: QVKIECYUJHTRKK-UHFFFAOYSA-N
Formula: C14H11NS2
SMILES: Cc1ccc(Sc2ccccc2N=C=S)cc1
Mol. weight [g/mol]: 257.37
CAS: 81431-97-2

Physical Properties

Property code	Value	Unit	Source
hf	443.77	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.881		Crippen Method
mcvol	194.680	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
tb	797.77	K	Joback Method
tc	1092.02	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81431972&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