Acetamide, N-(2-iodo-4-methylphenyl)-2-phenylthio-

Inchi: InChI=1S/C15H14INOS/c1-11-7-8-14(13(16)9-11)17-15(18)10-19-12-5-3-2-4-6-12/h2-9H

InchiKey: MNHFJTCEGYXIOL-UHFFFAOYSA-N

Formula: C15H14INOS

SMILES: Cc1ccc(N=C(O)CSc2ccccc2)c(I)c1

Mol. weight [g/mol]: 383.25

Physical Properties

Property code	Value	Unit	Source
hf	136.13	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.980		Crippen Method
mcvol	228.410	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	936.58	K	Joback Method
tc	1203.65	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=U307211&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature