

4-Iodophenyl isothiocyanate

Inchi: InChI=1S/C7H4INS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InchiKey: SNLGBRZZFRSXHA-UHFFFAOYSA-N
Formula: C7H4INS
SMILES: S=C=Nc1ccc(I)cc1
Mol. weight [g/mol]: 261.08
CAS: 2059-76-9

Physical Properties

Property code	Value	Unit	Source
hf	398.19	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.026		Crippen Method
mcpvol	129.280	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	630.31	K	Joback Method
tc	931.44	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=C2059769&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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