3-Iodothiophene

Other names:	Thiophene, 3-iodo-
Inchi:	InChI=1S/C4H3IS/c5-4-1-2-6-3-4/h1-3H
InchiKey:	WGKRMQIQXMJVFZ-UHFFFAOYSA-N
Formula:	C4H3IS
SMILES:	Ic1ccsc1
Mol. weight [g/mol]:	210.04
CAS:	10486-61-0

Physical Properties

Property code	Value	Unit	Source
ie	8.46	eV	NIST Webbook
log10ws	-2.38		Crippen Method
logp	2.353		Crippen Method
mcvol	89.930	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	1.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10486610&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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