

Thiophene, 2-iodo-

Other names:	2-Iodothiophene 2-Thienyl iodide «alpha»-Iodothiophene Â«alphaÂ»-Iodothiophene
Inchi:	InChI=1S/C4H3IS/c5-4-2-1-3-6-4/h1-3H
InchiKey:	ROIMNSWDOJCBFR-UHFFFAOYSA-N
Formula:	C4H3IS
SMILES:	Ic1cccs1
Mol. weight [g/mol]:	210.04
CAS:	3437-95-4

Physical Properties

Property code	Value	Unit	Source
ie	8.55 ± 0.05	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.52 ± 0.05	eV	NIST Webbook
log10ws	-2.38		Crippen Method
logp	2.353		Crippen Method
mvol	89.930	ml/mol	McGowan Method
tb	454.65 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	29.00	kJ/mol	353.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.04547e+01
Coeff. B	-1.07412e+04
Coeff. C	2.24114e+02
Temperature range (K), min.	308.50
Temperature range (K), max.	485.20

Sources

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=C3437954&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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