1-IODONAPHTHALENE

Other names:	1-Iodonapthalene
	1-Naphthyl iodide
	Iodonaphthalene
	naphthalene, 1-iodo-
	«alpha»-Iodonaphthalene
Inchi:	InChI=1S/C10H7I/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	NHPPIJMARIVBGU-UHFFFAOYSA-N
Formula:	C10H7I
SMILES:	Ic1cccc2ccccc12
Mol. weight [g/mol]:	254.07
CAS:	90-14-2

Physical Properties

Property code	Value	Unit	Source
af	0.3408		Cheméo Relay (1.0)
chl	-5096.90 ± 6.30	kJ/mol	NIST Webbook
gf	300.87	kJ/mol	Joback Method
hf	234.00 ± 8.80	kJ/mol	NIST Webbook
hfl	162.00 ± 6.30	kJ/mol	NIST Webbook
hfus	16.73	kJ/mol	Joback Method
hvap	72.40 ± 5.90	kJ/mol	NIST Webbook
hvap	69.90 ± 0.30	kJ/mol	NIST Webbook
ie	8.03	eV	NIST Webbook
log10ws	-4.55		Aqueous Solubility Prediction Method
log10ws	-4.55		Estimated Solubility Method
logp	3.444		Crippen Method
mcvol	134.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1571.90		NIST Webbook
rinpol	1571.90		NIST Webbook
tb	575.20	K	NIST Webbook
tc	850.22	K	Cheméo Relay (1.0)
tf	280.00 ± 1.00	K	NIST Webbook
vc	0.475	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.99	J/mol×K	754.84	Joback Method
cpg	310.30	J/mol×K	846.27	Joback Method
cpg	302.96	J/mol×K	800.56	Joback Method
cpg	286.25	J/mol×K	709.13	Joback Method
cpg	254.13	J/mol×K	571.98	Joback Method
cpg	265.95	J/mol×K	617.70	Joback Method
cpg	276.61	J/mol×K	663.41	Joback Method
dvisc	0.0020777	Pa×s	332.16	Joback Method
dvisc	0.0013681	Pa×s	372.13	Joback Method
dvisc	0.0009769	Pa×s	412.10	Joback Method
dvisc	0.0007404	Pa×s	452.07	Joback Method
dvisc	0.0005870	Pa×s	492.04	Joback Method
dvisc	0.0004819	Pa×s	532.01	Joback Method
dvisc	0.0004067	Pa×s	571.98	Joback Method
hfust	15.91	kJ/mol	280.00	NIST Webbook
hfust	15.91	kJ/mol	280.00	NIST Webbook
hvapt	78.90	kJ/mol	374.50	NIST Webbook
hvapt	70.10	kJ/mol	298.15	Enthalpies of Vaporization and Sublimation of the Halogen-Substituted Aromatic Hydrocarbons at 298.15 K: Application of Solution Calorimetry Approach

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28130e+01
Coeff. B	-3.95428e+03
Coeff. C	-1.10607e+02
Temperature range (K), min.	426.31
Temperature range (K), max.	637.74

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

Cheméo Relay (1.0):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0, beta):

Enthalpies of Vaporization and Sublimation of the Halogen-Substituted Aromatic Hydrocarbons at 298.15 K: https://www.doi.org/10.1021/je5008795

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90142&Units=SI

Joback Method: Application of Solution Calorimetry Approach: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume