Benzenamine, 3-iodo-

Other names:	Aniline, m-iodo-
	m-Aminoiodobenzene
	m-Iodoaniline
	3-Iodoaniline
	3-I-C6H4NH2
Inchi:	InChI=1S/C6H6IN/c7-5-2-1-3-6(8)4-5/h1-4H,8H2
InchiKey:	FFCSRWGYGMRBGD-UHFFFAOYSA-N
Formula:	C6H6IN
SMILES:	Nc1cccc(I)c1
Mol. weight [g/mol]:	219.02
CAS:	626-01-7

Physical Properties

Property code	Value	Unit	Source
affp	878.70	kJ/mol	NIST Webbook
basg	846.80	kJ/mol	NIST Webbook
gf	226.99	kJ/mol	Joback Method
hf	168.55	kJ/mol	Joback Method
hfus	14.50	kJ/mol	NIST Webbook
hvap	67.50 ± 1.40	kJ/mol	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.873		Crippen Method
mcvol	107.440	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
rinpol	1358.90		NIST Webbook
rinpol	1358.90		NIST Webbook
tb	534.01	K	Joback Method
tc	803.38	K	Joback Method
tf	337.64	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	187.75	J/mol×K	534.01	Joback Method
cpg	196.92	J/mol×K	578.90	Joback Method
cpg	205.30	J/mol×K	623.80	Joback Method
cpg	212.94	J/mol×K	668.69	Joback Method
cpg	219.91	J/mol×K	713.59	Joback Method
cpg	226.26	J/mol×K	758.48	Joback Method
cpg	232.06	J/mol×K	803.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.70	K	2.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C626017&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume