Benzenamine, 2-iodo-

Other names:	2-iodoaniline
	Aniline, o-iodo-
	aniline, 2-iodo-
	o-Aminoiodobenzene
	o-iodoaniline
Inchi:	InChI=1S/C6H6IN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2
InchiKey:	UBPDKIDWEADHPP-UHFFFAOYSA-N
Formula:	C6H6IN
SMILES:	Nc1ccccc1I
Mol. weight [g/mol]:	219.02
CAS:	615-43-0

Physical Properties

Property code	Value	Unit	Source
gf	226.99	kJ/mol	Joback Method
hf	168.55	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hsub	81.30 ± 1.40	kJ/mol	NIST Webbook
hvap	51.90	kJ/mol	Joback Method
ie	8.35	eV	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
tb	534.01	K	Joback Method
tc	803.38	K	Joback Method
tf	337.64	K	Joback Method
tt	325.70	K	Measurement and Correlation of the Dissolution Equilibria of o-Iodoaniline and p-Iodoaniline in Pure Solvents
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
hfust	19.38	kJ/mol	329.60	NIST Webbook
hfust	13.95	kJ/mol	333.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of the Dissolution Equilibria of o-Iodoaniline and p-Iodoaniline in Pure Solvents:	https://www.doi.org/10.1021/acs.jced.7b00840
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=C615430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume