

Benzenamine, 4-iodo-

Other names:	4-iodoaniline Aniline, p-iodo- aniline, 4-iodo- benzanamine, 4-iodo- p-Aminophenyl iodide p-iodoaniline
Inchi:	InChI=1S/C6H6IN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2
InchiKey:	VLVCDUSVTXIWGW-UHFFFAOYSA-N
Formula:	C6H6IN
SMILES:	Nc1ccc(I)cc1
Mol. weight [g/mol]:	219.02
CAS:	540-37-4

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	84.80 ± 1.40	kJ/mol	NIST Webbook
hvap	51.90	kJ/mol	Joback Method
ie	7.51	eV	NIST Webbook
ie	7.70 ± 0.10	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
rinpol	1411.00		NIST Webbook
tb	534.01	K	Joback Method
tc	803.38	K	Joback Method
tf	337.64	K	Joback Method
tt	332.35	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	16.94	kJ/mol	336.00	NIST Webbook
hfust	15.10	kJ/mol	334.00	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>

Solubility Measurement and Phase
Equilibrium Modeling of
2-Aminobenzamide in 15 Pure
Solvents:

<https://www.doi.org/10.1021/acs.jced.9b00350>

https://en.wikipedia.org/wiki/Joback_method

Joback Method:
McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C540374&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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