

N-(4-Iodophenyl)acetamide

Other names:	4'-Iodoacetanilide 4-Iodoacetanilide Acetamide, N-(4-iodophenyl)- Acetanilide, 4'-iodo- p-Iodoacetanilide
Inchi:	InChI=1S/C8H8INO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)
InchiKey:	SIULLDWIXYYVCU-UHFFFAOYSA-N
Formula:	C8H8INO
SMILES:	CC(=O)Nc1ccc(I)cc1
Mol. weight [g/mol]:	261.06
CAS:	622-50-4

Physical Properties

Property code	Value	Unit	Source
gf	137.85	kJ/mol	Joback Method
hf	34.37	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
ie	7.87 ± 0.03	eV	NIST Webbook
log10ws	-3.25		Aqueous Solubility Prediction Method
logp	2.250		Crippen Method
mvol	137.190	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	611.28	K	Joback Method
tc	865.69	K	Joback Method
tf	379.51	K	Joback Method
vc	0.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.31	J/mol×K	611.28	Joback Method
cpg	286.82	J/mol×K	653.68	Joback Method

cpg	296.48	J/mol×K	696.08	Joback Method
cpg	305.32	J/mol×K	738.49	Joback Method
cpg	313.42	J/mol×K	780.89	Joback Method
cpg	320.84	J/mol×K	823.29	Joback Method
cpg	327.61	J/mol×K	865.69	Joback Method

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C622504&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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
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
vc:	Critical Volume

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