

p-Iodo-N,N-dimethylaniline

Other names:	Aniline, p-iodo-N,N-dimethyl- Benzenamine, 4-iodo-N,N-dimethyl- N,N-Dimethyl-4-iodoaniline
Inchi:	InChI=1S/C8H10IN/c1-10(2)8-5-3-7(9)4-6-8/h3-6H,1-2H3
InchiKey:	QYOPPZJZMFMBDN-UHFFFAOYSA-N
Formula:	C8H10IN
SMILES:	CN(C)c1ccc(I)cc1
Mol. weight [g/mol]:	247.08
CAS:	698-70-4

Physical Properties

Property code	Value	Unit	Source
gf	288.16	kJ/mol	Joback Method
hf	161.01	kJ/mol	Joback Method
hfus	17.56	kJ/mol	Joback Method
hvap	47.76	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.357		Crippen Method
mcvol	135.620	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	519.68	K	Joback Method
tc	763.68	K	Joback Method
tf	309.39	K	Joback Method
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.60	J/mol×K	519.68	Joback Method
cpg	268.40	J/mol×K	560.35	Joback Method
cpg	280.23	J/mol×K	601.01	Joback Method
cpg	291.13	J/mol×K	641.68	Joback Method
cpg	301.18	J/mol×K	682.34	Joback Method
cpg	310.44	J/mol×K	723.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C698704&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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