

3-Iodo-5-nitroaniline

Inchi:	InChI=1S/C6H5IN2O2/c7-4-1-5(8)3-6(2-4)9(10)11/h1-3H,8H2
InchiKey:	BKYNSFHBQVINES-UHFFFAOYSA-N
Formula:	C6H5IN2O2
SMILES:	<chem>Nc1cc(I)cc([N+](=O)[O-])c1</chem>
Mol. weight [g/mol]:	264.02
CAS:	10394-64-6

Physical Properties

Property code	Value	Unit	Source
gf	252.91	kJ/mol	Joback Method
hf	146.32	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.782		Crippen Method
mcvol	124.860	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	690.83	K	Joback Method
tc	985.39	K	Joback Method
tf	493.77	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.68	J/molxK	690.83	Joback Method
cpg	264.70	J/molxK	739.92	Joback Method
cpg	271.93	J/molxK	789.02	Joback Method
cpg	278.42	J/molxK	838.11	Joback Method
cpg	284.26	J/molxK	887.21	Joback Method
cpg	289.53	J/molxK	936.30	Joback Method
cpg	294.31	J/molxK	985.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10394646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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