

Benzene, 1-iodo-4-nitro-

Other names:	p-Iodonitrobenzene p-Nitroiodobenzene p-Nitrophenyl iodide 1-Iodo-4-nitrobenzene 4-Iodonitrobenzene 4-Nitroiodobenzene
Inchi:	InChI=1S/C6H4INO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H
InchiKey:	SCCCFNJTCDSLKY-UHFFFAOYSA-N
Formula:	C6H4INO2
SMILES:	O=[N+](O)c1ccc(I)cc1
Mol. weight [g/mol]:	249.01
CAS:	636-98-6

Physical Properties

Property code	Value	Unit	Source
gf	196.09	kJ/mol	Joback Method
hf	124.00	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
ie	9.24	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.199		Crippen Method
mcvol	114.880	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	613.32	K	Joback Method
tc	902.66	K	Joback Method
tf	446.00 ± 2.00	K	NIST Webbook
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.25	J/molxK	613.32	Joback Method
cpg	222.78	J/molxK	661.54	Joback Method

cpg	230.44	J/mol×K	709.77	Joback Method
cpg	237.31	J/mol×K	757.99	Joback Method
cpg	243.47	J/mol×K	806.21	Joback Method
cpg	249.00	J/mol×K	854.43	Joback Method
cpg	253.99	J/mol×K	902.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	562.20	K	103.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C636986&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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