1-iodo-4-nitrobenzene

Other names:	4-iodo-1-nitrobenzene
	4-iodonitrobenzene
	4-nitro-1-iodobenzene
	4-nitroiodobenzene
	4-nitrophenyl iodide
	benzene, 1-iodo-4-nitro-
	p-iodonitrobenzene
	p-nitroiodobenzene
	p-nitrophenyl iodide
Inchi:	InChI=1S/C6H4INO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H
InchiKey:	SCCCFNJTCDSLCY-UHFFFAOYSA-N
Formula:	C6H4INO2
SMILES:	O=[N+]([O-])c1ccc(I)cc1
Mol. weight [g/mol]:	249.01

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
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	397.99	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.25	J/mol×K	613.32	Joback Method

cpg	222.78	J/mol×K	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
hvapt	98.20	kJ/mol	298.15	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.51e-04	kPa	315.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.14e-04	kPa	313.17	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.52e-04	kPa	315.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.93e-04	kPa	317.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	2.30e-04	kPa	319.13	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	2.83e-04	kPa	321.10	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers

psub	3.59e-04	kPa	323.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	4.55e-04	kPa	325.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	5.52e-04	kPa	327.12	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	8.57e-04	kPa	331.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.04e-03	kPa	333.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	9.40e-05	kPa	311.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.21e-04	kPa	313.17	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	9.70e-05	kPa	311.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.79e-04	kPa	317.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers

psub	2.30e-04	kPa	319.13	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	2.82e-04	kPa	321.10	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	3.55e-04	kPa	323.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	4.51e-04	kPa	325.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	5.50e-04	kPa	327.12	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	6.72e-04	kPa	329.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	8.56e-04	kPa	331.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	1.04e-03	kPa	333.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	

psub	9.30e-05	kPa	311.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	1.18e-04	kPa	313.17	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	1.50e-04	kPa	315.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	1.79e-04	kPa	317.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	2.26e-04	kPa	319.13	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	2.77e-04	kPa	321.10	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	3.54e-04	kPa	323.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	4.36e-04	kPa	325.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	
psub	5.46e-04	kPa	327.12	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers	

psub	6.73e-04	kPa	329.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	8.30e-04	kPa	331.18	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
psub	1.02e-03	kPa	333.11	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers:	https://www.doi.org/10.1016/j.jct.2012.09.031
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume