Benzene, 1-iodo-3-nitro-

Other names:	1-iodo-3-nitrobenzene
	3-iodo-1-nitrobenzene
	3-iodonitrobenzene
	3-nitroiodobenzene
	3-nitrophenyl iodide
	m-iodonitrobenzene
	m-nitroiodobenzene
	m-nitrophenyl iodide
Inchi:	InChI=1S/C6H4INO2/c7-5-2-1-3-6(4-5)8(9)10/h1-4H
InchiKey:	CBYAZOKPJYBCHE-UHFFFAOYSA-N
Formula:	C6H4INO2
SMILES:	O=[N+]([O-])c1cccc(I)c1
Mol. weight [g/mol]:	249.01
CAS:	645-00-1

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	553.20	K	NIST Webbook
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
hsubt	83.00 ± 2.00	kJ/mol	351.00	NIST Webbook
hsubt	83.20 ± 1.20	kJ/mol	300.50	NIST Webbook
hvapt	89.40	kJ/mol	298.15	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	1.90	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C645001&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

hsubt: Enthalpy of sublimation at a given temperature

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