

Benzene, 1-iodo-2-nitro-

Other names:	1-Iodo-2-nitrobenzene 2-Iodonitrobenzene 2-Nitroiodobenzene 2-nitrophenyl iodide o-Iodonitrobenzene o-Nitroiodobenzene o-nitrophenyl iodide
Inchi:	InChI=1S/C6H4INO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H
InchiKey:	JXMZUNPWVXQADG-UHFFFAOYSA-N
Formula:	C6H4INO2
SMILES:	O=[N+]([O-])c1ccccc1I
Mol. weight [g/mol]:	249.01
CAS:	609-73-4

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	561.70	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/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
hvapt	89.90	kJ/mol	298.15	Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers
hvapt	59.90	kJ/mol	498.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	561.70	K	97.20	NIST Webbook
tbrp	435.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.74121e+01
Coeff. B	-7.20479e+03
Temperature range (K), min.	420.73
Temperature range (K), max.	595.41

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=C609734&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
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
pvap:	Vapor 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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