

4-CHLORO-3-NITROPHENOL

Other names:	Phenol, 4-chloro-3-nitro-
Inchi:	InChI=1S/C6H4ClNO3/c7-5-2-1-4(9)3-6(5)8(10)11/h1-3,9H
InchiKey:	JUIKCULGDIZNDI-UHFFFAOYSA-N
Formula:	C6H4ClNO3
SMILES:	O=[N+](O)c1cc(O)ccc1Cl
Mol. weight [g/mol]:	173.56

Physical Properties

Property code	Value	Unit	Source
hf	-122.84	kJ/mol	Cheméo Relay (1.0)
hfus	25.97	kJ/mol	Thermochemical Parameters of the Chloronitrophenol Isomers: A Combined Experimental and Theoretical Investigation
hsub	111.00 ± 3.30	kJ/mol	NIST Webbook
hvap	84.26	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-2.22		Cheméo Relay (1.0)
logp	1.954		Crippen Method
mcvol	107.170	ml/mol	McGowan Method
tb	553.05	K	Cheméo Relay (1.0)
tf	346.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.17	J/mol×K	638.23	Joback Method
cpg	243.62	J/mol×K	683.09	Joback Method
cpg	250.40	J/mol×K	727.95	Joback Method
cpg	256.64	J/mol×K	772.81	Joback Method
cpg	262.46	J/mol×K	817.67	Joback Method
cpg	267.97	J/mol×K	862.53	Joback Method
cpg	273.30	J/mol×K	907.39	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical Parameters of the Chloronitrophenol Isomers: A Critical Review of Experimental and Theoretical Investigation:	https://www.doi.org/10.1021/je6005218
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C610786&Units=SI
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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