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]: 173.55
CAS: 610-78-6

Physical Properties

Property code	Value	Unit	Source
gf	-28.58	kJ/mol	Joback Method
hf	-145.92	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hsub	111.00 ± 3.30	kJ/mol	NIST Webbook
hvap	65.88	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.954		Crippen Method
mcvol	107.170	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	638.23	K	Joback Method
tc	907.39	K	Joback Method
tf	481.57	K	Joback Method
vc	0.360	m3/kmol	Joback Method

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

hfust	25.97	kJ/mol	399.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C610786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume