4-chloro-3-nitroaniline

Inchi: InChI=1S/C6H5ClN2O2/c7-5-2-1-4(8)3-6(5)9(10)11/h1-3H,8H2
InchiKey: FOHHWGVAOVDVLP-UHFFFAOYSA-N
Formula: C6H5ClN2O2
SMILES: Nc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 172.57

Physical Properties

Property code	Value	Unit	Source
gf	182.86	kJ/mol	Joback Method
hf	53.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.830		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	635.12	K	Joback Method
tc	902.71	K	Joback Method
tf	347.90	K	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.10	J/mol×K	902.71	Joback Method
cpg	273.99	J/mol×K	813.51	Joback Method
cpg	267.52	J/mol×K	768.91	Joback Method
cpg	260.38	J/mol×K	724.32	Joback Method
cpg	252.54	J/mol×K	679.72	Joback Method
cpg	243.95	J/mol×K	635.12	Joback Method
cpg	279.84	J/mol×K	858.11	Joback Method

psub	3.96e-04	kPa	341.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.72e-04	kPa	333.26	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.62e-04	kPa	333.26	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.63e-04	kPa	333.26	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.05e-04	kPa	335.21	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.07e-04	kPa	335.21	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.05e-04	kPa	335.21	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.44e-04	kPa	337.16	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.55e-04	kPa	337.16	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	2.51e-04	kPa	337.16	Combined experimental and computational thermochemistry of isomers of chloronitroanilines

psub	3.16e-04	kPa	339.27	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	3.20e-04	kPa	339.27	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	3.19e-04	kPa	339.27	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	3.95e-04	kPa	341.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.30e-04	kPa	331.14	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	3.89e-04	kPa	341.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	4.71e-04	kPa	343.12	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	4.86e-04	kPa	343.12	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	4.80e-04	kPa	343.12	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	6.05e-04	kPa	345.25	Combined experimental and computational thermochemistry of isomers of chloronitroanilines

psub	6.08e-04	kPa	345.25	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	6.01e-04	kPa	345.25	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	7.55e-04	kPa	347.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	7.55e-04	kPa	347.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	7.41e-04	kPa	347.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	9.14e-04	kPa	349.13	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	9.26e-04	kPa	349.13	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	8.95e-04	kPa	349.13	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.32e-04	kPa	331.14	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.29e-04	kPa	331.14	Combined experimental and computational thermochemistry of isomers of chloronitroanilines

psub	1.05e-04	kPa	329.20	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.04e-04	kPa	329.20	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	1.06e-04	kPa	329.20	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	8.47e-05	kPa	327.27	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
psub	8.67e-05	kPa	327.27	Combined experimental and computational thermochemistry of isomers of chloronitroanilines
rhos	1180.00	kg/m3	298.15	Combined experimental and computational thermochemistry of isomers of chloronitroanilines

Sources

Combined experimental and computational thermochemistry of isomers of chloronitroanilines:	https://www.doi.org/10.1016/j.jct.2007.07.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume