4-Chloro-3-nitrobenzaldehyde

Other names: Benzaldehyde, 4-chloro-3-nitro-
Inchi: InChI=1S/C7H4ClNO3/c8-6-2-1-5(4-10)3-7(6)9(11)12/h1-4H
InchiKey: HETBKLHJEWXWBM-UHFFFAOYSA-N
Formula: C7H4ClNO3
SMILES: O=Cc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 185.56
CAS: 16588-34-4

Physical Properties

Property code	Value	Unit	Source
gf	25.31	kJ/mol	Joback Method
hf	-86.30	kJ/mol	Joback Method
hfus	25.00	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.061		Crippen Method
mcvol	116.960	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	634.13	K	Joback Method
tc	889.95	K	Joback Method
tf	435.64	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.66	J/mol×K	634.13	Joback Method
cpg	258.93	J/mol×K	676.77	Joback Method
cpg	266.50	J/mol×K	719.40	Joback Method
cpg	273.40	J/mol×K	762.04	Joback Method
cpg	279.66	J/mol×K	804.68	Joback Method
cpg	285.31	J/mol×K	847.32	Joback Method
cpg	290.40	J/mol×K	889.95	Joback Method

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=C16588344&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
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