Benzoic acid, 3-chloro-4-nitro-

Other names: 3-Chloro-4-nitrobenzoic acid
Inchi: InChI=1S/C7H4ClNO4/c8-5-3-4(7(10)11)1-2-6(5)9(12)13/h1-3H,(H,10,11)
InchiKey: TZPGGFYKIOBMCN-UHFFFAOYSA-N
Formula: C7H4ClNO4
SMILES: O=C(O)c1ccc([N+](=O)[O-])c(Cl)c1
Mol. weight [g/mol]: 201.56
CAS: 39608-47-4

Physical Properties

Property code	Value	Unit	Source
gf	-140.91	kJ/mol	Joback Method
hf	-265.53	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.946		Crippen Method
mcvol	122.830	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	731.52	K	Joback Method
tc	968.96	K	Joback Method
tf	183.50 ± 1.50	K	NIST Webbook
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.94	J/mol×K	731.52	Joback Method
cpg	290.51	J/mol×K	771.09	Joback Method
cpg	296.51	J/mol×K	810.67	Joback Method
cpg	301.95	J/mol×K	850.24	Joback Method
cpg	306.87	J/mol×K	889.81	Joback Method
cpg	311.30	J/mol×K	929.39	Joback Method
cpg	315.25	J/mol×K	968.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39608474&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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