Benzene, 1-chloro-2-methyl-4-nitro-

Other names: 2-Chloro-5-nitrotoluene
Inchi: InChI=1S/C7H6ClNO2/c1-5-4-6(9(10)11)2-3-7(5)8/h2-4H,1H3
InchiKey: BGDCQZFFNFXYQC-UHFFFAOYSA-N
Formula: C7H6ClNO2
SMILES: Cc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]: 171.58
CAS: 13290-74-9

Physical Properties

Property code	Value	Unit	Source
gf	124.83	kJ/mol	Joback Method
hf	-0.72	kJ/mol	Joback Method
hfus	22.71	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.557		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	585.47	K	Joback Method
tc	840.46	K	Joback Method
tf	393.64	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.86	J/mol×K	585.47	Joback Method
cpg	251.78	J/mol×K	627.97	Joback Method
cpg	260.95	J/mol×K	670.47	Joback Method
cpg	269.40	J/mol×K	712.97	Joback Method
cpg	277.17	J/mol×K	755.46	Joback Method
cpg	284.29	J/mol×K	797.96	Joback Method
cpg	290.80	J/mol×K	840.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	521.20	K	94.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13290749&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume