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

Other names:	Toluene, 4-chloro-3-nitro-
	3-Nitro-4-chlorotoluene
	4-Chloro-3-nitrotoluene
	4,3-Chloronitrotoluene
	1-Chloro-4-methyl-2-nitrobenzene
	2-Chloro-5-methylnitrobenzene
Inchi:	InChI=1S/C7H6ClNO2/c1-5-2-3-6(8)7(4-5)9(10)11/h2-4H,1H3
InchiKey:	NWESJZZPAJGHRZ-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	Cc1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	171.58
CAS:	89-60-1

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
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2039.00		NIST Webbook
tb	585.47	K	Joback Method
tc	840.46	K	Joback Method
tf	280.33 ± 0.30	K	NIST Webbook
tf	280.40 ± 0.20	K	NIST Webbook
tf	279.90 ± 0.25	K	NIST Webbook
tf	280.11 ± 0.35	K	NIST Webbook
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	533.20	K	99.30	NIST Webbook
tbrp	391.20	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89601&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume