

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

Other names:	Toluene, 2-chloro-4-nitro- o-Chloro-p-nitrotoluol 2-Chloro-4-nitrotoluene 3-Chloro-4-methylnitrobenzene 2,4-Chloronitrotoluene 2-Chlor-4-nitrotoluen
Inchi:	InChI=1S/C7H6ClNO2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,1H3
InchiKey:	LLYXJBROWQDVMU-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	<chem>Cc1ccc([N+](=O)[O-])cc1Cl</chem>
Mol. weight [g/mol]:	171.58
CAS:	121-86-8

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	1316.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1316.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1965.00		NIST Webbook
tb	585.47	K	Joback Method
tc	840.46	K	Joback Method
tf	393.64	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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