

4-Chloro-2-nitrotoluene

Other names:	4,2-Chloronitrotoluene Benzene, 4-chloro-1-methyl-2-nitro- p-Chloro-o-nitrotoluene Toluene, 4-chloro-2-nitro- 2-Nitro-4-chlorotoluene
Inchi:	InChI=1S/C7H6ClNO2/c1-5-2-3-6(8)4-7(5)9(10)11/h2-4H,1H3
InchiKey:	SQFLFRQWPBEDHM-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	<chem>Cc1ccc(Cl)cc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	171.58
CAS:	89-59-8

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
ripol	1268.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1915.00		NIST Webbook
tb	585.47	K	Joback Method
tc	840.46	K	Joback Method
tf	309.95 ± 0.20	K	NIST Webbook
tf	309.12 ± 0.40	K	NIST Webbook
vc	0.451	m ³ /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	512.70	K	95.70	NIST Webbook
tbrp	513.20	K	96.00	NIST Webbook
tbrp	388.70	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=C89598&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

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