

Benzene, 1-(chloromethyl)-3-nitro-

Other names:	«alpha»-Chloro-m-nitrotoluene m-Nitrobenzyl chloride 3-Nitrobenzyl chloride Toluene, «alpha»-chloro-m-nitro- Toluene, alpha-chloro-m-nitro- «alpha»-chloro-3-nitrotoluene
Inchi:	InChI=1S/C7H6ClNO2/c8-5-6-2-1-3-7(4-6)9(10)11/h1-4H,5H2
InchiKey:	APGGSERFJKEWFG-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	O=[N+]([O-])c1cccc(CCl)c1
Mol. weight [g/mol]:	171.58
CAS:	619-23-8

Physical Properties

Property code	Value	Unit	Source
gf	134.46	kJ/mol	Joback Method
hf	10.75	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	55.09	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.334		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	580.49	K	Joback Method
tc	834.39	K	Joback Method
tf	381.12	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.16	J/mol×K	580.49	Joback Method
cpg	253.38	J/mol×K	622.81	Joback Method
cpg	262.77	J/mol×K	665.12	Joback Method

cpg	271.39	J/mol×K	707.44	Joback Method
cpg	279.27	J/mol×K	749.76	Joback Method
cpg	286.47	J/mol×K	792.08	Joback Method
cpg	293.02	J/mol×K	834.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	0.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619238&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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