Benzene, 1-(chloromethyl)-4-nitro-

Other names:	Toluene, «alpha»-chloro-p-nitro- «alpha»-Chloro-p-nitrotoluene p-Nitrobenzyl chloride 1-(Chloromethyl)-4-nitrobenzene 4-(Chloromethyl)nitrobenzene 4-Nitrobenzyl chloride p-(Chloromethyl)nitrobenzene Toluene, alpha-chloro-p-nitro NSC 9803 «alpha»-chloro-4-nitrotoluene
Inchi:	InChI=1S/C7H6ClNO2/c8-5-6-1-3-7(4-2-6)9(10)11/h1-4H,5H2
InchiKey:	KGCNHWXDPDPSBV-UHFFFAOYSA-N
Formula:	C7H6ClNO2
SMILES:	O=[N+]([O-])c1ccc(CCl)cc1
Mol. weight [g/mol]:	171.58
CAS:	100-14-1

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	m3/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

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100141&Units=SI

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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume