Benzene, 1-chloro-2-nitro-4-(trifluoromethyl)-

Other names: (3-Nitro-4-chlorophenyl)trifluoromethane
1-Chloro-4-trifluoromethyl-2-nitrobenzene
2-Chloro-5-(trifluoromethyl)nitrobenzene
2-NITRO-4-TRIFLUOROMETHYLCHLOROBENZENE
2-Nitro-4-(trifluoromethyl)chlorobenzene
3-NITRO-4-CHLORO-A,A,A-TRIFLUOROTOLUENE
3-Nitro-4-(chloro)trifluoromethylbenzene
3-Nitro-4-chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
3-Nitro-4-chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
3-Nitro-4-chlorobenzotrifluoride
4-CHLORO-3-NITROBENZOTRIFLUORIDE
4-Chloro-3-nitro-1-(trifluoromethyl)benzene
4-Chloro-3-nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
4-Chloro-3-nitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
4-Chloro-3-nitrobenzylidyne fluoride
4-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-3-nitrotoluene
4-Chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-3-nitrotoluene
Benzotrifluoride, 4-chloro-3-nitro-
NSC 8760
Toluene, 4-chloro-3-nitro-«alpha»,«alpha»,«alpha»-trifluoro-
Toluene, 4-chloro-3-nitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-
Toluene, 4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-3-nitro-
Toluene, 4-chloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-3-nitro-
UN 2307

Inchi: InChI=1S/C7H3ClF3NO2/c8-5-2-1-4(7(9,10)11)3-6(5)12(13)14/h1-3H

InchiKey: TZGFQIXRVUHDLE-UHFFFAOYSA-N

Formula: C7H3ClF3NO2

SMILES: O=[N+]([O-])c1cc(C(F)(F)F)ccc1Cl

Mol. weight [g/mol]: 225.55

CAS: 121-17-5

Physical Properties

Property code	Value	Unit	Source
chs	-3229.50 ± 9.00	kJ/mol	NIST Webbook
gf	-456.76	kJ/mol	Joback Method
hf	-597.80	kJ/mol	Joback Method

hfs	-330.80 ± 0.92	kJ/mol	NIST Webbook
hfus	24.53	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.267		Crippen Method
mcvol	120.700	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	495.20	K	NIST Webbook
tc	812.52	K	Joback Method
tf	397.83	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.79	J/mol×K	580.05	Joback Method
cpg	279.64	J/mol×K	618.79	Joback Method
cpg	287.69	J/mol×K	657.54	Joback Method
cpg	295.00	J/mol×K	696.28	Joback Method
cpg	301.61	J/mol×K	735.03	Joback Method
cpg	307.61	J/mol×K	773.77	Joback Method
cpg	313.02	J/mol×K	812.52	Joback Method
hvapt	57.60	kJ/mol	426.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.50 ± 0.50	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51029e+01

Coeff. B	-4.36147e+03
Coeff. C	-7.91610e+01
Temperature range (K), min.	373.55
Temperature range (K), max.	524.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.42593e+02
Coeff. B	-1.30588e+04
Coeff. C	-1.83270e+01
Coeff. D	8.61235e-06
Temperature range (K), min.	293.15
Temperature range (K), max.	686.00

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1802

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121175&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1802

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

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume