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

Other names:	Toluene, 2-chloro-«alpha»,«alpha»,«alpha»-trifluoro-5-nitro-
	2-(Trifluoromethyl)-4-nitrochlorobenzene
	3-(Trifluoromethyl)-4-chloronitrobenzene
	4-Chloro-3-(trifluoromethyl)nitrobenzene
	2-Chloro-5-nitrobenzotrifluoride
	2-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-5-nitrotoluene
Inchi:	InChI=1S/C7H3ClF3NO2/c8-6-2-1-4(12(13)14)3-5(6)7(9,10)11/h1-3H
InchiKey:	HQROXDLWVGFPDE-UHFFFAOYSA-N
Formula:	C7H3ClF3NO2
SMILES:	O=[N+]([O-])c1ccc(Cl)c(C(F)(F)F)c1
Mol. weight [g/mol]:	225.55
CAS:	777-37-7

Physical Properties

Property code	Value	Unit	Source
gf	-456.76	kJ/mol	Joback Method
hf	-597.80	kJ/mol	Joback Method
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	505.20	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	58.10	kJ/mol	436.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	1.30	NIST Webbook
tbrp	375.50 ± 0.50	K	0.70	NIST Webbook
tbrp	389.50 ± 1.50	K	2.40	NIST Webbook

Sources

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=C777377&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

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