Benzene, 2-chloro-1,3-dinitro-5-(trifluoromethyl)-

Other names: Benzene, 2-chloro-5-(trifluoromethyl)-1,3-dinitro-
Trifluoromethyl-3,5-dinitro-4-chlorobenzene
3,5-Dinitro-4-chlorobenzotrifluoride
4-Chloro-3,5-dinitrobenzotrifluoride
Toluene, 4-chloro-«alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitro-
1-Chloro-2,6-dinitro-4-(trifluoromethyl)benzene
2-Chloro-1,3-dinitro-5-(trifluoromethyl)benzene
2,6-Dinitro-4-trifluoromethylchlorobenzene
4-(Trifluoromethyl)-2,6-dinitrochlorobenzene
4-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitrotoluene
4-Chloro-3,5-dinitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
Toluene, 4-chloro-3,5-dinitro-«alpha»,«alpha»,«alpha»-trifluoro-
Benzotrifluoride, 4-chloro-3,5-dinitro-
3,5-Dinitro-4-chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
Benzene, 1-chloro-2,6-dinitro-4-trifluoromethyl
NSC 88274
Chloralin

Inchi: InChI=1S/C7H2ClF3N2O4/c8-6-4(12(14)15)1-3(7(9,10)11)2-5(6)13(16)17/h1-2H

InchiKey: HFHAVERNVFNSHL-UHFFFAOYSA-N

Formula: C7H2ClF3N2O4

SMILES: O=[N+]([O-])c1cc(C(F)(F)F)cc([N+](=O)[O-])c1Cl

Mol. weight [g/mol]: 270.55

CAS: 393-75-9

Physical Properties

Property code	Value	Unit	Source
chs	-3087.00 ± 10.00	kJ/mol	NIST Webbook
gf	-430.84	kJ/mol	Joback Method
hf	-620.03	kJ/mol	Joback Method
hfs	-260.00 ± 0.88	kJ/mol	NIST Webbook
hfus	35.50	kJ/mol	Joback Method
hvap	69.26	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.175		Crippen Method
mcvol	138.120	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	736.87	K	Joback Method

tc	991.26	K	Joback Method
tf	553.96	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.87	J/mol×K	736.87	Joback Method
cpg	349.95	J/mol×K	779.27	Joback Method
cpg	356.27	J/mol×K	821.67	Joback Method
cpg	361.91	J/mol×K	864.07	Joback Method
cpg	366.94	J/mol×K	906.46	Joback Method
cpg	371.43	J/mol×K	948.86	Joback Method
cpg	375.45	J/mol×K	991.26	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C393759&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

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
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