4-CHLORO-3-NITROBENZYLIDYNE TRIFLUORIDE

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-chlorobenzotrifluoride
4-Chloro-3-nitro-1-(trifluoromethyl)benzene
4-Chloro-3-nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
4-Chloro-3-nitrobenzotrifluoride
4-Chloro-3-nitrobenzylidyne fluoride
4-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-3-nitrotoluene
Benzotrifluoride, 4-chloro-3-nitro-
NSC 8760
Toluene, 4-chloro-3-nitro-«alpha»,«alpha»,«alpha»-trifluoro-
Toluene, 4-chloro-«alpha»,«alpha»,«alpha»-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
hfs	-330.80 ± 0.92	kJ/mol	NIST Webbook
hfus	24.53	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.77		Cheméo Relay (1.0)
logp	3.267		Crippen Method
mcvol	120.700	ml/mol	McGowan Method
tb	495.20	K	NIST Webbook
tf	311.71	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121175&Units=SI
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1802
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1802
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point