3-CHLOROBENZOTRIFLUORIDE

Other names:	1-Chloro-3-(trifluoromethyl)benzene 3-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene Toluene, m-chloro-«alpha»,«alpha»,«alpha»-trifluoro- UN 2234 m-Chloro-«alpha»,«alpha»,«alpha»-trifluorotoluene m-Chlorobenzotrifluoride m-Trifluoromethylphenyl chloride meta(Trifluoromethyl)chlorobenzene
Inchi:	InChI=1S/C7H4ClF3/c8-6-3-1-2-5(4-6)7(9,10)11/h1-4H
InchiKey:	YTCGOUNVIAWCMG-UHFFFAOYSA-N
Formula:	C7H4ClF3
SMILES:	FC(F)(F)c1cccc(Cl)c1
Mol. weight [g/mol]:	180.56
CAS:	98-15-7

Physical Properties

Property code	Value	Unit	Source
hf	-606.15	kJ/mol	Cheméo Relay (1.0)
hfus	13.56	kJ/mol	Joback Method
hvap	43.56	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-2.83		Cheméo Relay (1.0)
logp	3.359		Crippen Method
mcvol	103.280	ml/mol	McGowan Method
rinpol	834.50		NIST Webbook
rinpol	834.50		NIST Webbook
tb	411.00 ± 2.00	K	NIST Webbook
tb	410.70	K	NIST Webbook
tc	616.32	K	Cheméo Relay (1.0)
tf	260.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.34	J/mol×K	423.23	Joback Method
cpg	201.41	J/mol×K	456.51	Joback Method
cpg	210.74	J/mol×K	489.78	Joback Method
cpg	219.39	J/mol×K	523.06	Joback Method
cpg	227.38	J/mol×K	556.34	Joback Method
cpg	234.75	J/mol×K	589.61	Joback Method
cpg	241.55	J/mol×K	622.89	Joback Method
hvapt	43.00	kJ/mol	356.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42628e+01
Coeff. B	-3.37458e+03
Coeff. C	-6.07510e+01
Temperature range (K), min.	302.22
Temperature range (K), max.	437.74

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98157&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point