3,4-Dichlorobenzotrifluoride

Other names:	3,4-dichloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	3,4-dichloro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
	Benzene, 1,2-dichloro-4-(trifluoromethyl)-
Inchi:	InChI=1S/C7H3Cl2F3/c8-5-2-1-4(3-6(5)9)7(10,11)12/h1-3H
InchiKey:	XILPLWOGHPSJBK-UHFFFAOYSA-N
Formula:	C7H3Cl2F3
SMILES:	FC(F)(F)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	215.00
CAS:	328-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-504.24	kJ/mol	Joback Method
hf	-602.78	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	39.80	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	4.012		Crippen Method
mcvol	115.520	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	446.70	K	NIST Webbook
tb	446.50 ± 0.50	K	NIST Webbook
tc	673.39	K	Joback Method
tf	284.14	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.20	J/mol×K	465.64	Joback Method
cpg	224.05	J/mol×K	500.26	Joback Method
cpg	232.21	J/mol×K	534.89	Joback Method
cpg	239.74	J/mol×K	569.51	Joback Method
cpg	246.66	J/mol×K	604.14	Joback Method

cpg	253.01	J/mol×K	638.76	Joback Method
cpg	258.84	J/mol×K	673.39	Joback Method
hvapt	44.10	kJ/mol	403.00	NIST Webbook
hvapt	41.80	kJ/mol	365.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74419e+01
Coeff. B	-6.07136e+03
Coeff. C	2.68530e+01
Temperature range (K), min.	327.07
Temperature range (K), max.	473.65

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C328847&Units=SI

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume