Benzene, 1-fluoro-4-(trifluoromethyl)-

Other names:	1-Fluoro-4-(trifluoromethyl)benzene
	4-Fluorobenzotrifluoride
	NSC 88289
	Toluene, p,«alpha»,«alpha»,«alpha»-tetrafluoro-
	Toluene, p,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-tetrafluoro-
	p,«alpha»,«alpha»,«alpha»-Tetrafluorotoluene
	p,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Tetrafluorotoluene
	p-(Trifluoromethyl)fluorobenzene
	p-Fluorobenzotrifluoride
	p-Fluorotrifluoromethylbenzene
	«alpha»,«alpha»,«alpha»,4-tetrafluorotoluene
	«alpha»,«alpha»,«alpha»,p-Tetrafluorotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,4-tetrafluorotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,p-Tetrafluorotoluene
Inchi:	InChI=1S/C7H4F4/c8-6-3-1-5(2-4-6)7(9,10)11/h1-4H
InchiKey:	UNNNAIWPDLRVRN-UHFFFAOYSA-N
Formula:	C7H4F4
SMILES:	Fc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	164.10
CAS:	402-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-665.56	kJ/mol	Joback Method
hf	-755.94	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	29.55	kJ/mol	Joback Method
ie	9.98	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.845		Crippen Method
mcvol	92.810	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	376.70	K	NIST Webbook
tb	375.90	K	NIST Webbook
tc	566.36	K	Joback Method
tf	212.37	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.11	J/mol×K	536.14	Joback Method
cpg	174.38	J/mol×K	385.07	Joback Method
cpg	184.55	J/mol×K	415.28	Joback Method
cpg	194.08	J/mol×K	445.50	Joback Method
cpg	203.00	J/mol×K	475.71	Joback Method
cpg	211.34	J/mol×K	505.93	Joback Method
cpg	226.36	J/mol×K	566.36	Joback Method
hvapt	35.80	kJ/mol	333.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64671e+01
Coeff. B	-4.03068e+03
Coeff. C	-2.35950e+01
Temperature range (K), min.	272.72
Temperature range (K), max.	384.91

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C402448&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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
ie:	Ionization energy
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