Benzene, 1-fluoro-2-(trifluoromethyl)-

Other names:	o-Fluorobenzotrifluoride
	2-Fluorobenzotrifluoride
	o,«alpha»,«alpha»,«alpha»-Tetrafluorotoluene
	Toluene, «alpha»,«alpha»,«alpha»,o-tetrafluoro-
	Toluene, o,«alpha»,«alpha»,«alpha»-tetrafluoro-
	1-Fluoro-2-(trifluoromethyl)benzene
	o,alpha,alpha,alpha-Tetrafluorotoluene
	NSC 10314
	«alpha»,«alpha»,«alpha»,2-tetrafluorotoluene
Inchi:	InChI=1S/C7H4F4/c8-6-4-2-1-3-5(6)7(9,10)11/h1-4H
InchiKey:	BGVGHYOIWIALFF-UHFFFAOYSA-N
Formula:	C7H4F4
SMILES:	Fc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	164.10
CAS:	392-85-8

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	38.10	kJ/mol	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	387.50 ± 0.50	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	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	219.11	J/mol×K	536.14	Joback Method
cpg	226.36	J/mol×K	566.36	Joback Method
hfust	10.70	kJ/mol	222.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	100.00	NIST Webbook

Sources

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=C392858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume