Benzene, (fluoromethyl)-

Other names:	(Fluoromethyl)benzene
	Benzyl fluoride
	Toluene, «alpha»-fluoro-
	Toluene, Â«alphaÂ»-fluoro-
	«alpha»-Fluorotoluene
	Â«alphaÂ»-Fluorotoluene
Inchi:	InChI=1S/C7H7F/c8-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	MBXXQYJBFRRFCK-UHFFFAOYSA-N
Formula:	C7H7F
SMILES:	FCc1ccccc1
Mol. weight [g/mol]:	110.13
CAS:	350-50-5

Physical Properties

Property code	Value	Unit	Source
chl	-3762.83 ± 0.68	kJ/mol	NIST Webbook
gf	-74.34	kJ/mol	Joback Method
hf	-126.27 ± 0.73	kJ/mol	NIST Webbook
hfl	-172.59 ± 0.68	kJ/mol	NIST Webbook
hfus	11.01	kJ/mol	Joback Method
hvap	46.32 ± 0.26	kJ/mol	NIST Webbook
hvap	46.50	kJ/mol	NIST Webbook
hvap	46.30 ± 0.30	kJ/mol	NIST Webbook
hvap	44.50 ± 0.40	kJ/mol	NIST Webbook
hvap	46.20 ± 0.30	kJ/mol	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.20		Crippen Method
logp	2.156		Crippen Method
mcvol	87.500	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	864.00		NIST Webbook

tb	413.00	K	NIST Webbook
tb	412.00	K	NIST Webbook
tc	584.96	K	Joback Method
tf	210.70 ± 0.30	K	NIST Webbook
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.45	J/mol×K	385.51	Joback Method
cpg	157.30	J/mol×K	418.75	Joback Method
cpg	167.55	J/mol×K	451.99	Joback Method
cpg	177.20	J/mol×K	485.23	Joback Method
cpg	186.30	J/mol×K	518.48	Joback Method
cpg	194.85	J/mol×K	551.72	Joback Method
cpg	202.89	J/mol×K	584.96	Joback Method
hvapt	43.70	kJ/mol	353.50	NIST Webbook
hvapt	44.30	kJ/mol	327.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.00	K	100.00	NIST Webbook
tbrp	313.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46318e+01
Coeff. B	-3.56474e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	304.52
Temperature range (K), max.	438.48

Sources

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=C350505&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume