Benzene, pentafluoro(trifluoromethyl)-

Other names:	(Trifluoromethyl)pentafluorobenzene OCTAFLUOROTOLUENE Pentafluoro(trifluoro-methyl)benzene Perfluorotoluene Toluene, octafluoro- pentafluoro(trifluoromethyl)benzene
Inchi:	InChI=1S/C7F8/c8-2-1(7(13,14)15)3(9)5(11)6(12)4(2)10
InchiKey:	USPWUOFNOTUBAD-UHFFFAOYSA-N
Formula:	C7F8
SMILES:	Fc1c(F)c(F)c(C(F)(F)F)c(F)c1F
Mol. weight [g/mol]:	236.06
CAS:	434-64-0

Physical Properties

Property code	Value	Unit	Source
af	0.4750		KDB
ea	0.86 ± 0.11	eV	NIST Webbook
ea	1.70 ± 0.30	eV	NIST Webbook
gf	-1483.32	kJ/mol	Joback Method
hf	-1269.40 ± 7.80	kJ/mol	NIST Webbook
hfl	-1311.10 ± 7.80	kJ/mol	NIST Webbook
hfus	23.21	kJ/mol	Joback Method
hvap	41.60 ± 0.20	kJ/mol	NIST Webbook
hvap	40.40	kJ/mol	NIST Webbook
hvap	40.50 ± 0.20	kJ/mol	NIST Webbook
hvap	41.60 ± 0.20	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.40 ± 0.10	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-4.23		Crippen Method
logp	3.401		Crippen Method
mcvol	99.890	ml/mol	McGowan Method
pc	2705.00 ± 4.00	kPa	NIST Webbook
pc	2680.00	kPa	NIST Webbook
pc	2705.00	kPa	KDB
rhoc	551.91 ± 0.54	kg/m3	NIST Webbook

sl	360.10	J/mol×K	NIST Webbook
sl	355.50	J/mol×K	NIST Webbook
tb	377.00 ± 1.00	K	NIST Webbook
tb	377.20	K	NIST Webbook
tb	377.73	K	KDB
tc	534.47	K	KDB
tc	534.47 ± 0.05	K	NIST Webbook
tc	534.40	K	NIST Webbook
tc	534.47 ± 0.20	K	NIST Webbook
tf	207.50	K	KDB
tt	207.69 ± 0.02	K	NIST Webbook
tt	207.62 ± 0.02	K	NIST Webbook
vc	0.428	m3/kmol	KDB
zc	0.2605260		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.09	J/mol×K	528.47	Joback Method
cpg	237.61	J/mol×K	503.19	Joback Method
cpg	231.84	J/mol×K	477.91	Joback Method
cpg	225.78	J/mol×K	452.63	Joback Method
cpg	219.42	J/mol×K	427.35	Joback Method
cpg	248.31	J/mol×K	553.75	Joback Method
cpg	212.76	J/mol×K	402.07	Joback Method
cpl	262.30	J/mol×K	298.15	NIST Webbook
cpl	266.40	J/mol×K	298.15	NIST Webbook
hfust	11.49	kJ/mol	207.69	NIST Webbook
hfust	11.49	kJ/mol	207.00	NIST Webbook
hfust	11.49	kJ/mol	207.00	NIST Webbook
hfust	11.58	kJ/mol	207.62	NIST Webbook
hvapt	40.00	kJ/mol	334.50	NIST Webbook
hvapt	40.90	kJ/mol	330.50	NIST Webbook
kvisc	0.0000005	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000006	m2/s	303.15	Viscosities of Liquid Fluorocompounds

kvisc	0.0000006	m2/s	298.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	318.15	Viscosities of Liquid Fluorocompounds
pvap	21.31	kPa	333.93	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.95	kPa	293.20	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	13.38	kPa	323.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	10.69	kPa	318.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	8.43	kPa	313.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	3.87	kPa	298.28	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	6.54	kPa	308.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	5.09	kPa	303.18	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	2.18	kPa	288.23	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	16.86	kPa	328.45	Densities and Vapor Pressures of Highly Fluorinated Compounds
sfust	55.32	J/mol×K	207.69	NIST Webbook
srf	0.02	N/m	313.75	Surface Tension of Liquid Fluorocompounds

srf	0.02	N/m	308.55	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	298.25	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	293.15	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	287.15	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	318.85	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	303.35	Surface Tension of Liquid Fluorocompounds

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1687.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
Densities and Vapor Pressures of Highly Fluorinated Compounds:	https://www.doi.org/10.1021/je050056e
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C434640&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
ea:	Electron affinity
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
kvisc:	Kinematic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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