

Benzene, pentachlorofluoro-

Other names:	Fluoropentachlorobenzene Pentachlorofluorobenzene 1-Fluoropentachlorobenzene
Inchi:	InChI=1S/C6Cl5F/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	HGLRKPSTNKQNIS-UHFFFAOYSA-N
Formula:	C6Cl5F
SMILES:	Fc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	268.33
CAS:	319-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-190.56	kJ/mol	Joback Method
hf	-262.80	kJ/mol	Joback Method
hfus	27.46	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	5.093		Crippen Method
mcvol	134.610	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	574.68	K	Joback Method
tc	814.17	K	Joback Method
tf	396.59	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.93	J/mol×K	574.68	Joback Method
cpg	213.58	J/mol×K	614.59	Joback Method
cpg	217.93	J/mol×K	654.51	Joback Method
cpg	221.99	J/mol×K	694.42	Joback Method
cpg	225.74	J/mol×K	734.34	Joback Method
cpg	229.21	J/mol×K	774.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C319879&Units=SI
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

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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