Benzene, pentafluoro-2-propenyl-

Other names: Benzene, allylpentafluoro-
Allylpentafluorobenzene
Pentafluoroallylbenzene
Inchi: InChI=1S/C9H5F5/c1-2-3-4-5(10)7(12)9(14)8(13)6(4)11/h2H,1,3H2
InchiKey: YBDBTBVNQQBHGJ-UHFFFAOYSA-N
Formula: C9H5F5
SMILES: C=CCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 208.13
CAS: 1736-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-797.05	kJ/mol	Joback Method
hf	-905.03	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	36.46	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.111		Crippen Method
mcvol	118.460	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
tb	421.70	K	NIST Webbook
tb	421.50 ± 0.50	K	NIST Webbook
tc	618.08	K	Joback Method
tf	281.40	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.22	J/mol×K	449.93	Joback Method
cpg	252.66	J/mol×K	477.96	Joback Method
cpg	260.78	J/mol×K	505.98	Joback Method
cpg	268.58	J/mol×K	534.01	Joback Method
cpg	276.07	J/mol×K	562.03	Joback Method

cpg	283.25	J/mol×K	590.06	Joback Method
cpg	290.13	J/mol×K	618.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1736603&Units=SI

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