

Benzene, ethenylpentafluoro-

Other names:	Pentafluorostyrene 2,3,4,5,6-Pentafluorostyrene Styrene, 2,3,4,5,6-pentafluoro- Vinylpentafluorobenzene
Inchi:	InChI=1S/C8H3F5/c1-2-3-4(9)6(11)8(13)7(12)5(3)10/h2H,1H2
InchiKey:	LVJZCPNIJXVIAT-UHFFFAOYSA-N
Formula:	C8H3F5
SMILES:	C=Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	194.10
CAS:	653-34-9

Physical Properties

Property code	Value	Unit	Source
gf	-805.47	kJ/mol	Joback Method
hf	-884.39	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	34.23	kJ/mol	Joback Method
ie	9.18 ± 0.02	eV	NIST Webbook
log10ws	-3.95		Crippen Method
logp	3.025		Crippen Method
mcvol	104.370	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	412.50 ± 0.50	K	NIST Webbook
tc	596.17	K	Joback Method
tf	270.13	K	Joback Method
vc	0.447	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.41	J/mol×K	427.05	Joback Method
cpg	213.65	J/mol×K	455.24	Joback Method
cpg	220.62	J/mol×K	483.42	Joback Method
cpg	227.32	J/mol×K	511.61	Joback Method

cpg	233.76	J/mol×K	539.80	Joback Method
cpg	239.94	J/mol×K	567.99	Joback Method
cpg	245.86	J/mol×K	596.17	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	6.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653349&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

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
ie:	Ionization energy
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

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