Benzene, (chloromethyl)pentafluoro-

Other names: «alpha»-Chloro-2,3,4,5,6-pentafluorotoluene
(chloromethyl)pentafluorobenzene
Inchi: InChI=1S/C7H2ClF5/c8-1-2-3(9)5(11)7(13)6(12)4(2)10/h1H2
InchiKey: ZLNVRXFZTPRLIK-UHFFFAOYSA-N
Formula: C7H2ClF5
SMILES: Fc1c(F)c(F)c(CCl)c(F)c1F
Mol. weight [g/mol]: 216.54
CAS: 653-35-0

Physical Properties

Property code	Value	Unit	Source
gf	-913.66	kJ/mol	Joback Method
hf	-1004.92	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	37.06	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.121		Crippen Method
mcvol	106.820	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	444.92	K	Joback Method
tc	618.30	K	Joback Method
tf	290.54	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.96	J/mol×K	444.92	Joback Method
cpg	213.37	J/mol×K	473.82	Joback Method
cpg	219.54	J/mol×K	502.71	Joback Method
cpg	225.48	J/mol×K	531.61	Joback Method
cpg	231.19	J/mol×K	560.51	Joback Method
cpg	236.67	J/mol×K	589.40	Joback Method
cpg	241.91	J/mol×K	618.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653350&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
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