1-Fluoropentachlorobenzene

Other names: 1-Fluoropentachlorobenzene
Fluoropentachlorobenzene
Pentachlorofluorobenzene
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

Physical Properties

Property code	Value	Unit	Source
af	0.4727		Cheméo Relay (1.0)
hf	-175.67	kJ/mol	Cheméo Relay (1.0)
hfus	27.46	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-6.18		Cheméo Relay (1.0)
logp	5.093		Crippen Method
mcvol	134.610	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	550.43	K	Cheméo Relay (1.0)
tc	798.47	K	Cheméo Relay (1.0)
tf	428.65	K	Cheméo Relay (1.0)
vc	0.509	m3/kmol	Cheméo Relay (1.0)

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

cpg	232.39	J/mol×K	814.17	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume