1-CHLORO-2,3,5,6-TETRAFLUOROBENZENE

Other names: Benzene,3-chloro-1,2,4,5-tetrafluoro-
Inchi: InChI=1S/C6HClF4/c7-4-5(10)2(8)1-3(9)6(4)11/h1H
InchiKey: QLDHPPIOYFTGAJ-UHFFFAOYSA-N
Formula: C6HClF4
SMILES: Fc1cc(F)c(F)c(Cl)c1F
Mol. weight [g/mol]: 184.52

Physical Properties

Property code	Value	Unit	Source
af	0.3762		Cheméo Relay (1.0)
hf	-611.91	kJ/mol	Cheméo Relay (1.0)
hfus	20.30	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	2.896		Crippen Method
mcvol	90.960	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	400.98	K	Cheméo Relay (1.0)
tc	594.88	K	Cheméo Relay (1.0)
tf	254.30	K	Cheméo Relay (1.0)
vc	0.357	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.68	J/mol×K	417.79	Joback Method
cpg	168.45	J/mol×K	448.24	Joback Method
cpg	173.98	J/mol×K	478.68	Joback Method
cpg	179.27	J/mol×K	509.13	Joback Method
cpg	184.33	J/mol×K	539.58	Joback Method
cpg	189.17	J/mol×K	570.02	Joback Method
cpg	193.78	J/mol×K	600.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1835616&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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