

Benzene, 1,2-dichloro-3,4,5,6-tetrafluoro-

Other names:	1,2-Dichlorotetrafluorobenzene Benzene, 1,2-dichlorotetrafluoro-
Inchi:	InChI=1S/C6Cl2F4/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	OZRCFSKDIYWITR-UHFFFAOYSA-N
Formula:	C6Cl2F4
SMILES:	Fc1c(F)c(F)c(Cl)c(Cl)c1F
Mol. weight [g/mol]:	218.96
CAS:	1198-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-739.20	kJ/mol	Joback Method
hf	-803.91	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	40.04	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.550		Crippen Method
mcvol	103.200	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	460.20	K	Joback Method
tc	650.88	K	Joback Method
tf	308.60	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.91	J/mol×K	460.20	Joback Method
cpg	186.98	J/mol×K	491.98	Joback Method
cpg	191.83	J/mol×K	523.76	Joback Method
cpg	196.48	J/mol×K	555.54	Joback Method
cpg	200.92	J/mol×K	587.32	Joback Method
cpg	205.16	J/mol×K	619.10	Joback Method
cpg	209.19	J/mol×K	650.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1198590&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1662.mol

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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