

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

Other names:	Benzene, 1,3-dichlorotetrafluoro- 1,3-Dichloro-2,4,5,6-tetrafluorobenzene 1,3-Dichlorotetrafluorobenzene 2,4,5,6-Tetrafluoro-1,3-dichlorobenzene
Inchi:	InChI=1S/C6Cl2F4/c7-1-3(9)2(8)5(11)6(12)4(1)10
InchiKey:	LFJIYWQWRQWQC-UHFFFAOYSA-N
Formula:	C6Cl2F4
SMILES:	Fc1c(F)c(Cl)c(F)c(Cl)c1F
Mol. weight [g/mol]:	218.96
CAS:	1198-61-4

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	424.20	K	NIST Webbook
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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1198614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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