1,3-Dichloro-2,4,6-trifluorobenzene

Other names: Benzene,2,4-dichloro-1,3,5-trifluoro-
Inchi: InChI=1S/C6HCl2F3/c7-4-2(9)1-3(10)5(8)6(4)11/h1H
InchiKey: UOGVNYNJSZHQCN-UHFFFAOYSA-N
Formula: C6HCl2F3
SMILES: Fc1cc(F)c(Cl)c(F)c1Cl
Mol. weight [g/mol]: 200.97
CAS: 2368-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-534.76	kJ/mol	Joback Method
hf	-596.33	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
ie	9.37 ± 0.02	eV	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.411		Crippen Method
mcvol	101.430	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	434.70	K	NIST Webbook
tc	655.71	K	Joback Method
tf	295.49	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.88	J/mol×K	455.95	Joback Method
cpg	179.63	J/mol×K	489.24	Joback Method
cpg	185.11	J/mol×K	522.54	Joback Method
cpg	190.31	J/mol×K	555.83	Joback Method
cpg	195.25	J/mol×K	589.12	Joback Method
cpg	199.92	J/mol×K	622.42	Joback Method
cpg	204.34	J/mol×K	655.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2368538&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
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