1-Chloro-2,4-difluorobenzene

Other names: Benzene,1-chloro-2,4-difluoro-
Inchi: InChI=1S/C6H3ClF2/c7-5-2-1-4(8)3-6(5)9/h1-3H
InchiKey: AJCSNHQKXUSMMY-UHFFFAOYSA-N
Formula: C6H3ClF2
SMILES: Fc1ccc(Cl)c(F)c1
Mol. weight [g/mol]: 148.54
CAS: 1435-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-308.76	kJ/mol	Joback Method
hf	-361.54	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	35.30	kJ/mol	Joback Method
ie	9.17 ± 0.02	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.618		Crippen Method
mcvol	87.420	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	400.20	K	NIST Webbook
tc	610.29	K	Joback Method
tf	239.94	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.97	J/mol×K	409.29	Joback Method
cpg	152.39	J/mol×K	442.79	Joback Method
cpg	159.40	J/mol×K	476.29	Joback Method
cpg	166.03	J/mol×K	509.79	Joback Method
cpg	172.28	J/mol×K	543.29	Joback Method
cpg	178.17	J/mol×K	576.79	Joback Method
cpg	183.71	J/mol×K	610.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435445&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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