2,6-Dichloro-4-fluorophenol

Other names: Phenol, 2,6-dichloro-4-fluoro-
Inchi: InChI=1S/C6H3Cl2FO/c7-4-1-3(9)2-5(8)6(4)10/h1-2,10H
InchiKey: BOJVIFKSTRCIRJ-UHFFFAOYSA-N
Formula: C6H3Cl2FO
SMILES: Oc1c(Cl)cc(F)cc1Cl
Mol. weight [g/mol]: 180.99
CAS: 392-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-280.50	kJ/mol	Joback Method
hf	-358.48	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	53.52	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.838		Crippen Method
mcvol	103.760	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	528.07	K	Joback Method
tc	762.73	K	Joback Method
tf	380.99	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.86	J/mol×K	528.07	Joback Method
cpg	200.40	J/mol×K	567.18	Joback Method
cpg	206.37	J/mol×K	606.29	Joback Method
cpg	211.83	J/mol×K	645.40	Joback Method
cpg	216.87	J/mol×K	684.51	Joback Method
cpg	221.55	J/mol×K	723.62	Joback Method
cpg	225.94	J/mol×K	762.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C392712&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
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