Benzene, 1,2-dichloro-3-fluoro-

Inchi: InChI=1S/C6H3Cl2F/c7-4-2-1-3-5(9)6(4)8/h1-3H
InchiKey: NPXCSDPOOVOVDQ-UHFFFAOYSA-N
Formula: C6H3Cl2F
SMILES: Fc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 164.99
CAS: 36556-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-125.88	kJ/mol	Joback Method
hf	-181.17	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	40.50	kJ/mol	Joback Method
ie	9.29 ± 0.02	eV	NIST Webbook
log10ws	-3.17		Crippen Method
logp	3.132		Crippen Method
mcvol	97.890	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	447.45	K	Joback Method
tc	667.64	K	Joback Method
tf	269.27	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.45	J/mol×K	447.45	Joback Method
cpg	164.82	J/mol×K	484.15	Joback Method
cpg	171.73	J/mol×K	520.85	Joback Method
cpg	178.19	J/mol×K	557.55	Joback Method
cpg	184.23	J/mol×K	594.25	Joback Method
cpg	189.87	J/mol×K	630.94	Joback Method
cpg	195.11	J/mol×K	667.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36556500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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