1-Chloro-2,6-dibromo-4-fluorobenzene

Other names: Benzene, 1,3-dibromo-2-chloro-5-fluoro-
Inchi: InChI=1S/C6H2Br2ClF/c7-4-1-3(10)2-5(8)6(4)9/h1-2H
InchiKey: PZKDJJMHRYNBOR-UHFFFAOYSA-N
Formula: C6H2Br2ClF
SMILES: Fc1cc(Br)c(Cl)c(Br)c1
Mol. weight [g/mol]: 288.34
CAS: 179897-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-94.94	kJ/mol	Joback Method
hf	-124.24	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	49.65	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.004		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
tb	547.32	K	Joback Method
tc	797.03	K	Joback Method
tf	371.47	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.79	J/mol×K	547.32	Joback Method
cpg	194.93	J/mol×K	588.94	Joback Method
cpg	200.55	J/mol×K	630.56	Joback Method
cpg	205.72	J/mol×K	672.17	Joback Method
cpg	210.45	J/mol×K	713.79	Joback Method
cpg	214.80	J/mol×K	755.41	Joback Method
cpg	218.80	J/mol×K	797.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C179897906&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