5-Fluoro-1,2,3-tribromobenzene

Other names: Benzene, 1,2,3-tribromo-5-fluoro-
Inchi: InChI=1S/C6H2Br3F/c7-4-1-3(10)2-5(8)6(4)9/h1-2H
InchiKey: FMIFEFSTHLAERU-UHFFFAOYSA-N
Formula: C6H2Br3F
SMILES: Fc1cc(Br)c(Br)c(Br)c1
Mol. weight [g/mol]: 332.79
CAS: 576-82-9

Physical Properties

Property code	Value	Unit	Source
gf	-68.69	kJ/mol	Joback Method
hf	-82.17	kJ/mol	Joback Method
hfus	23.11	kJ/mol	Joback Method
hvap	51.70	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.113		Crippen Method
mcvol	125.910	ml/mol	McGowan Method
pc	5519.63	kPa	Joback Method
tb	576.05	K	Joback Method
tc	836.41	K	Joback Method
tf	401.35	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.34	J/mol×K	576.05	Joback Method
cpg	200.25	J/mol×K	619.44	Joback Method
cpg	205.61	J/mol×K	662.84	Joback Method
cpg	210.50	J/mol×K	706.23	Joback Method
cpg	214.97	J/mol×K	749.63	Joback Method
cpg	219.08	J/mol×K	793.02	Joback Method
cpg	222.88	J/mol×K	836.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C576829&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
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