1,4-Dibromo-2-fluorobenzene

Inchi: InChI=1S/C6H3Br2F/c7-4-1-2-5(8)6(9)3-4/h1-3H
InchiKey: WNSNPGHNIJOOPM-UHFFFAOYSA-N
Formula: C6H3Br2F
SMILES: Fc1cc(Br)ccc1Br
Mol. weight [g/mol]: 253.89
CAS: 1435-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-73.38	kJ/mol	Joback Method
hf	-97.03	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.351		Crippen Method
mcvol	108.410	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	489.00	K	NIST Webbook
tb	489.20	K	NIST Webbook
tc	748.62	K	Joback Method
tf	329.03	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.55	J/mol×K	504.91	Joback Method
cpg	178.77	J/mol×K	545.53	Joback Method
cpg	185.41	J/mol×K	586.15	Joback Method
cpg	191.50	J/mol×K	626.77	Joback Method
cpg	197.08	J/mol×K	667.39	Joback Method
cpg	202.20	J/mol×K	708.00	Joback Method
cpg	206.91	J/mol×K	748.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435525&Units=SI

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