1-Bromo-2,3,4,6-tetrafluorobenzene

Other names: Benzene, 2-bromo-1,3,4,5-tetrafluoro-
2-bromo-1,3,4,5-tetrafluorobenzene
Inchi: InChI=1S/C6HBrF4/c7-4-2(8)1-3(9)5(10)6(4)11/h1H
InchiKey: AHJRONLVHNFUNH-UHFFFAOYSA-N
Formula: C6HBrF4
SMILES: Fc1cc(F)c(Br)c(F)c1F
Mol. weight [g/mol]: 228.97
CAS: 1559-86-0

Physical Properties

Property code	Value	Unit	Source
gf	-691.39	kJ/mol	Joback Method
hf	-734.63	kJ/mol	Joback Method
hfus	21.39	kJ/mol	Joback Method
hvap	37.04	kJ/mol	Joback Method
ie	9.46 ± 0.02	eV	NIST Webbook
log10ws	-3.96		Crippen Method
logp	3.006		Crippen Method
mcvol	96.220	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	415.20	K	NIST Webbook
tc	639.98	K	Joback Method
tf	296.04	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.51	J/mol×K	446.52	Joback Method
cpg	175.39	J/mol×K	478.76	Joback Method
cpg	180.97	J/mol×K	511.01	Joback Method
cpg	186.26	J/mol×K	543.25	Joback Method
cpg	191.28	J/mol×K	575.49	Joback Method
cpg	196.03	J/mol×K	607.73	Joback Method

cpg	200.51	J/mol×K	639.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1559860&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
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