1-Bromo-2,3,5,6-tetrafluorobenzene

Other names:	1-Bromo-2,3,5,6-tetrafluorbenzene
	2,3,5,6-Tetrafluorobromo benzene
	Benzene, 3-bromo-1,2,4,5-tetrafluoro-
Inchi:	InChI=1S/C6HBrF4/c7-4-5(10)2(8)1-3(9)6(4)11/h1H
InchiKey:	YHAFCGSUIAFUCX-UHFFFAOYSA-N
Formula:	C6HBrF4
SMILES:	Fc1cc(F)c(F)c(Br)c1F
Mol. weight [g/mol]:	228.97
CAS:	1559-88-2

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	9.45 ± 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	416.50	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

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=C1559882&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

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