3-Bromo-5-fluorobenzotrifluoride

Inchi: InChI=1S/C7H3BrF4/c8-5-1-4(7(10,11)12)2-6(9)3-5/h1-3H
InchiKey: LIGBGEJPUQBLTG-UHFFFAOYSA-N
Formula: C7H3BrF4
SMILES: Fc1cc(Br)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 243.00
CAS: 130723-13-6

Physical Properties

Property code	Value	Unit	Source
gf	-660.87	kJ/mol	Joback Method
hf	-741.08	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	36.65	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.607		Crippen Method
mcvol	110.310	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	456.21	K	Joback Method
tc	657.47	K	Joback Method
tf	284.69	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.05	J/mol×K	456.21	Joback Method
cpg	219.04	J/mol×K	489.75	Joback Method
cpg	227.34	J/mol×K	523.30	Joback Method
cpg	235.00	J/mol×K	556.84	Joback Method
cpg	242.05	J/mol×K	590.38	Joback Method
cpg	248.54	J/mol×K	623.93	Joback Method
cpg	254.51	J/mol×K	657.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C130723136&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