1-Bromo-2,4,6-trifluorobenzene

Other names: Benzene, 2-bromo-1,3,5-trifluoro-
Inchi: InChI=1S/C6H2BrF3/c7-6-4(9)1-3(8)2-5(6)10/h1-2H
InchiKey: PZBSPSOGEVCRQI-UHFFFAOYSA-N
Formula: C6H2BrF3
SMILES: Fc1cc(F)c(Br)c(F)c1
Mol. weight [g/mol]: 210.98
CAS: 2367-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-486.95	kJ/mol	Joback Method
hf	-527.05	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	37.20	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.866		Crippen Method
mcvol	94.450	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	442.27	K	Joback Method
tc	645.14	K	Joback Method
tf	282.93	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.19	J/mol×K	442.27	Joback Method
cpg	167.83	J/mol×K	476.08	Joback Method
cpg	174.10	J/mol×K	509.89	Joback Method
cpg	180.01	J/mol×K	543.70	Joback Method
cpg	185.57	J/mol×K	577.51	Joback Method
cpg	190.79	J/mol×K	611.33	Joback Method
cpg	195.70	J/mol×K	645.14	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=C2367762&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
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