2-Fluoro-4-bromobenzaldehyde

Other names: 4-Bromo-2-fluorobenzaldehyde
Benzaldehyde, 4-bromo-2-fluoro-
Inchi: InChI=1S/C7H4BrFO/c8-6-2-1-5(4-10)7(9)3-6/h1-4H
InchiKey: UPCARQPLANFGQJ-UHFFFAOYSA-N
Formula: C7H4BrFO
SMILES: O=Cc1ccc(Br)cc1F
Mol. weight [g/mol]: 203.01
CAS: 57848-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-178.80	kJ/mol	Joback Method
hf	-229.58	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	47.11	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.401		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	510.29	K	Joback Method
tc	736.98	K	Joback Method
tf	322.50	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.83	J/mol×K	510.29	Joback Method
cpg	201.87	J/mol×K	548.07	Joback Method
cpg	209.35	J/mol×K	585.85	Joback Method
cpg	216.30	J/mol×K	623.63	Joback Method
cpg	222.76	J/mol×K	661.42	Joback Method
cpg	228.74	J/mol×K	699.20	Joback Method
cpg	234.28	J/mol×K	736.98	Joback Method

Sources

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=C57848461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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