4-Bromo-2-fluoroanisole

Other names: Benzene, 4-bromo-2-fluoro-1-methoxy-
Inchi: InChI=1S/C7H6BrFO/c1-10-7-3-2-5(8)4-6(7)9/h2-4H,1H3
InchiKey: DWNXGZBXFDNKOR-UHFFFAOYSA-N
Formula: C7H6BrFO
SMILES: COc1ccc(Br)cc1F
Mol. weight [g/mol]: 205.02
CAS: 2357-52-0

Physical Properties

Property code	Value	Unit	Source
gf	-184.28	kJ/mol	Joback Method
hf	-276.22	kJ/mol	Joback Method
hfus	16.70	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.597		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	484.05	K	Joback Method
tc	704.15	K	Joback Method
tf	302.73	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.16	J/mol×K	484.05	Joback Method
cpg	211.35	J/mol×K	520.73	Joback Method
cpg	220.05	J/mol×K	557.42	Joback Method
cpg	228.28	J/mol×K	594.10	Joback Method
cpg	236.05	J/mol×K	630.78	Joback Method
cpg	243.36	J/mol×K	667.47	Joback Method
cpg	250.22	J/mol×K	704.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	0.90	NIST Webbook

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=C2357520&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume