4-Bromo-2-fluorocinnamic acid

Other names: 2-Propenoic acid, 3-(4-bromo-2-fluorophenyl)-
Inchi: InChI=1S/C9H6BrFO2/c10-7-3-1-6(8(11)5-7)2-4-9(12)13/h1-5H,(H,12,13)/b4-2+
InchiKey: SVJGKQYKYNDYMU-DUXPYHPUSA-N
Formula: C9H6BrFO2
SMILES: O=C(O)C=Cc1ccc(Br)cc1F
Mol. weight [g/mol]: 245.04
CAS: 149947-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-247.96	kJ/mol	Joback Method
hf	-332.87	kJ/mol	Joback Method
hfus	26.58	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.686		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	657.60	K	Joback Method
tc	873.37	K	Joback Method
tf	408.71	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.88	J/mol×K	657.60	Joback Method
cpg	303.69	J/mol×K	693.56	Joback Method
cpg	310.95	J/mol×K	729.52	Joback Method
cpg	317.69	J/mol×K	765.48	Joback Method
cpg	323.98	J/mol×K	801.44	Joback Method
cpg	329.84	J/mol×K	837.40	Joback Method
cpg	335.32	J/mol×K	873.37	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=C149947193&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