5-Fluoro-2-methylbenzoic acid

Other names: Benzoic acid, 5-fluoro-2-methyl-
Inchi: InChI=1S/C8H7FO2/c1-5-2-3-6(9)4-7(5)8(10)11/h2-4H,1H3,(H,10,11)
InchiKey: JVBLXLBINTYFPR-UHFFFAOYSA-N
Formula: C8H7FO2
SMILES: Cc1ccc(F)cc1C(=O)O
Mol. weight [g/mol]: 154.14
CAS: 33184-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-350.92	kJ/mol	Joback Method
hf	-455.78	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.832		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	564.40	K	Joback Method
tc	763.02	K	Joback Method
tf	342.72	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.15	J/mol×K	564.40	Joback Method
cpg	251.74	J/mol×K	597.50	Joback Method
cpg	259.85	J/mol×K	630.61	Joback Method
cpg	267.50	J/mol×K	663.71	Joback Method
cpg	274.70	J/mol×K	696.82	Joback Method
cpg	281.46	J/mol×K	729.92	Joback Method
cpg	287.81	J/mol×K	763.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33184166&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