4-Fluoro-2-methoxyphenol, acetate

Inchi: InChI=1S/C9H9FO3/c1-6(11)13-8-4-3-7(10)5-9(8)12-2/h3-5H,1-2H3
InchiKey: AGAAKZLWQYHEGL-UHFFFAOYSA-N
Formula: C9H9FO3
SMILES: COc1cc(F)ccc1OC(C)=O
Mol. weight [g/mol]: 184.16

Physical Properties

Property code	Value	Unit	Source
gf	-415.68	kJ/mol	Joback Method
hf	-588.63	kJ/mol	Joback Method
hfus	19.38	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.760		Crippen Method
mcvol	128.990	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1255.90		NIST Webbook
rinpol	1255.90		NIST Webbook
tb	539.94	K	Joback Method
tc	745.43	K	Joback Method
tf	337.63	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.79	J/mol×K	539.94	Joback Method
cpg	297.93	J/mol×K	574.19	Joback Method
cpg	308.58	J/mol×K	608.44	Joback Method
cpg	318.72	J/mol×K	642.69	Joback Method
cpg	328.36	J/mol×K	676.94	Joback Method
cpg	337.47	J/mol×K	711.19	Joback Method
cpg	346.05	J/mol×K	745.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352864&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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