Benzoic acid, 2-fluoro-, ethyl ester

Other names:	Ethyl o-fluorobenzoate
	Ethyl 2-fluorobenzoate
	Benzoic acid, o-fluoro-, ethyl ester
	2-Fluorobenzoic acid, ethyl ester
Inchi:	InChI=1S/C9H9FO2/c1-2-12-9(11)7-5-3-4-6-8(7)10/h3-6H,2H2,1H3
InchiKey:	RUWPGPOBTHOLHF-UHFFFAOYSA-N
Formula:	C9H9FO2
SMILES:	CCOC(=O)c1ccccc1F
Mol. weight [g/mol]:	168.16
CAS:	443-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-301.05	kJ/mol	Joback Method
hf	-444.94	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.002		Crippen Method
mcvol	123.120	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1223.00		NIST Webbook
tb	512.54	K	Joback Method
tc	718.86	K	Joback Method
tf	302.88	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.57	J/mol×K	512.54	Joback Method
cpg	276.18	J/mol×K	546.93	Joback Method
cpg	287.19	J/mol×K	581.31	Joback Method
cpg	297.62	J/mol×K	615.70	Joback Method

cpg	307.46	J/mol×K	650.08	Joback Method
cpg	316.72	J/mol×K	684.47	Joback Method
cpg	325.43	J/mol×K	718.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C443265&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

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