Methyl 2-fluorobenzoate

Other names:	Benzoic acid, 2-fluoro-, methyl ester
	o-Fluorobenzoic acid, methyl ester
	Benzoic acid, o-fluoro-, methyl ester
	Methyl o-fluorobenzoate
	2-Fluorobenzoic acid, methyl ester
Inchi:	InChI=1S/C8H7FO2/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5H,1H3
InchiKey:	QAFJIJWLEBLXHH-UHFFFAOYSA-N
Formula:	C8H7FO2
SMILES:	COC(=O)c1ccccc1F
Mol. weight [g/mol]:	154.14
CAS:	394-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-309.47	kJ/mol	Joback Method
hf	-424.30	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.612		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	1151.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1151.00		NIST Webbook
tb	489.66	K	Joback Method
tc	699.06	K	Joback Method
tf	291.61	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.54	J/mol×K	489.66	Joback Method

cpg	233.02	J/mol×K	524.56	Joback Method
cpg	242.97	J/mol×K	559.46	Joback Method
cpg	252.38	J/mol×K	594.36	Joback Method
cpg	261.27	J/mol×K	629.26	Joback Method
cpg	269.64	J/mol×K	664.16	Joback Method
cpg	277.50	J/mol×K	699.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394354&Units=SI

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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