

2-Fluorobenzoic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C14H11FO2/c1-10-5-4-6-11(9-10)17-14(16)12-7-2-3-8-13(12)15/h2-9H,1H3
InchiKey:	VMZWTGUJXJPIEG-UHFFFAOYSA-N
Formula:	C14H11FO2
SMILES:	<chem>Cc1cccc(OC(=O)c2ccccc2F)c1</chem>
Mol. weight [g/mol]:	230.23

Physical Properties

Property code	Value	Unit	Source
gf	-156.17	kJ/mol	Joback Method
hf	-323.08	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.353		Crippen Method
mvol	169.810	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1751.00		NIST Webbook
tb	658.60	K	Joback Method
tc	891.72	K	Joback Method
tf	398.17	K	Joback Method
vc	0.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.07	J/mol×K	658.60	Joback Method
cpg	436.20	J/mol×K	697.45	Joback Method
cpg	449.28	J/mol×K	736.31	Joback Method
cpg	461.35	J/mol×K	775.16	Joback Method
cpg	472.44	J/mol×K	814.01	Joback Method
cpg	482.59	J/mol×K	852.87	Joback Method
cpg	491.82	J/mol×K	891.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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