3-Fluorobenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H11FO2/c1-10-4-2-7-13(8-10)17-14(16)11-5-3-6-12(15)9-11/h2-9H,1H3
InchiKey: UIXLXXNLGFASHO-UHFFFAOYSA-N
Formula: C14H11FO2
SMILES: Cc1cccc(OC(=O)c2cccc(F)c2)c1
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
mcvol	169.810	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	658.60	K	Joback Method
tc	891.72	K	Joback Method
tf	398.17	K	Joback Method
vc	0.645	m3/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

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=U307725&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