3-Fluorobenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C16H15FO3/c1-11(2)19-14-8-3-4-9-15(14)20-16(18)12-6-5-7-13(17)10-12/h3-1

InchiKey: XDJUPJJTOYOWQQ-UHFFFAOYSA-N

Formula: C16H15FO3

SMILES: CC(C)Oc1ccccc1OC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 274.29

Physical Properties

Property code	Value	Unit	Source
gf	-246.77	kJ/mol	Joback Method
hf	-501.86	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.832		Crippen Method
mcvol	203.860	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1829.00		NIST Webbook
tb	726.34	K	Joback Method
tc	952.21	K	Joback Method
tf	427.94	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.83	J/mol×K	726.34	Joback Method
cpg	566.75	J/mol×K	763.98	Joback Method
cpg	580.53	J/mol×K	801.63	Joback Method
cpg	593.20	J/mol×K	839.27	Joback Method
cpg	604.78	J/mol×K	876.92	Joback Method
cpg	615.29	J/mol×K	914.56	Joback Method
cpg	624.75	J/mol×K	952.21	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=U299059&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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