2-Fluorobenzoic acid, 2,3-dimethylphenyl ester

Inchi: InChI=1S/C15H13FO2/c1-10-6-5-9-14(11(10)2)18-15(17)12-7-3-4-8-13(12)16/h3-9H,1-2

InchiKey: IAXVIYGMQYIILF-UHFFFAOYSA-N

Formula: C15H13FO2

SMILES: Cc1cccc(OC(=O)c2ccccc2F)c1C

Mol. weight [g/mol]: 244.26

Physical Properties

Property code	Value	Unit	Source
gf	-157.38	kJ/mol	Joback Method
hf	-355.19	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.662		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1945.00		NIST Webbook
tb	686.46	K	Joback Method
tc	915.93	K	Joback Method
tf	421.96	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.83	J/mol×K	686.46	Joback Method
cpg	486.31	J/mol×K	724.71	Joback Method
cpg	499.74	J/mol×K	762.95	Joback Method
cpg	512.16	J/mol×K	801.20	Joback Method
cpg	523.61	J/mol×K	839.44	Joback Method
cpg	534.10	J/mol×K	877.69	Joback Method
cpg	543.67	J/mol×K	915.93	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=U354706&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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