4-Fluoro-2-trifluoromethylbenzoic acid, 4-isopropylphenyl ester

Inchi: InChI=1S/C17H14F4O2/c1-10(2)11-3-6-13(7-4-11)23-16(22)14-8-5-12(18)9-15(14)17(19

InchiKey: FIOIQCOHMQCPSL-UHFFFAOYSA-N

Formula: C17H14F4O2

SMILES: CC(C)c1ccc(OC(=O)c2ccc(F)cc2C(F)(F)F)cc1

Mol. weight [g/mol]: 326.29

Physical Properties

Property code	Value	Unit	Source
gf	-724.57	kJ/mol	Joback Method
hf	-998.83	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.187		Crippen Method
mcvol	217.390	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook
tb	726.36	K	Joback Method
tc	936.57	K	Joback Method
tf	433.69	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/mol×K	726.36	Joback Method
cpg	617.80	J/mol×K	761.39	Joback Method
cpg	630.73	J/mol×K	796.43	Joback Method
cpg	642.68	J/mol×K	831.46	Joback Method
cpg	653.70	J/mol×K	866.50	Joback Method
cpg	663.83	J/mol×K	901.53	Joback Method
cpg	673.13	J/mol×K	936.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343773&Units=SI
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

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