5-Fluoro-2-trifluoromethylbenzoic acid, isopropyl ester

Inchi: InChI=1S/C11H10F4O2/c1-6(2)17-10(16)8-5-7(12)3-4-9(8)11(13,14)15/h3-6H,1-2H3
InchiKey: QLLDUUJMNSCLEN-UHFFFAOYSA-N
Formula: C11H10F4O2
SMILES: CC(C)OC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 250.19

Physical Properties

Property code	Value	Unit	Source
gf	-877.87	kJ/mol	Joback Method
hf	-1100.05	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.410		Crippen Method
mcvol	156.610	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
tb	557.42	K	Joback Method
tc	746.37	K	Joback Method
tf	327.13	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.55	J/mol×K	557.42	Joback Method
cpg	394.97	J/mol×K	588.91	Joback Method
cpg	406.67	J/mol×K	620.40	Joback Method
cpg	417.68	J/mol×K	651.89	Joback Method
cpg	428.02	J/mol×K	683.38	Joback Method
cpg	437.71	J/mol×K	714.87	Joback Method
cpg	446.78	J/mol×K	746.37	Joback Method

Sources

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=U357623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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