2-Trifluorobenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H15F3O3/c1-11(2)22-14-9-5-6-10-15(14)23-16(21)12-7-3-4-8-13(12)17(18
InchiKey: RKUHEWWYEWWTCT-UHFFFAOYSA-N
Formula: C17H15F3O3
SMILES: CC(C)Oc1ccccc1OC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 324.29

Physical Properties

Property code	Value	Unit	Source
gf	-625.13	kJ/mol	Joback Method
hf	-923.47	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	66.74	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.712		Crippen Method
mcvol	221.490	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	744.53	K	Joback Method
tc	960.20	K	Joback Method
tf	442.81	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.58	J/mol×K	744.53	Joback Method
cpg	637.87	J/mol×K	780.47	Joback Method
cpg	651.04	J/mol×K	816.42	Joback Method
cpg	663.13	J/mol×K	852.36	Joback Method
cpg	674.19	J/mol×K	888.31	Joback Method
cpg	684.27	J/mol×K	924.25	Joback Method
cpg	693.41	J/mol×K	960.20	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=U299013&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