2,4,5-Trifluoro-3-methoxybenzoic acid, isopropyl ester

Inchi: InChI=1S/C11H11F3O3/c1-5(2)17-11(15)6-4-7(12)9(14)10(16-3)8(6)13/h4-5H,1-3H3
InchiKey: NWLHVQCFZQCHIA-UHFFFAOYSA-N
Formula: C11H11F3O3
SMILES: COc1c(F)c(F)cc(C(=O)OC(C)C)c1F
Mol. weight [g/mol]: 248.20

Physical Properties

Property code	Value	Unit	Source
gf	-810.16	kJ/mol	Joback Method
hf	-1050.35	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.678		Crippen Method
mcvol	160.710	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1376.00		NIST Webbook
tb	593.76	K	Joback Method
tc	781.69	K	Joback Method
tf	371.39	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.06	J/mol×K	593.76	Joback Method
cpg	405.76	J/mol×K	625.08	Joback Method
cpg	416.96	J/mol×K	656.40	Joback Method
cpg	427.65	J/mol×K	687.72	Joback Method
cpg	437.81	J/mol×K	719.04	Joback Method
cpg	447.44	J/mol×K	750.36	Joback Method
cpg	456.53	J/mol×K	781.69	Joback Method

Sources

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=U357606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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