2,5-Di(trifluoromethyl)benzoic acid, isopropyl ester

Inchi: InChI=1S/C12H10F6O2/c1-6(2)20-10(19)8-5-7(11(13,14)15)3-4-9(8)12(16,17)18/h3-6H,1

InchiKey: JBBBTQHHAVTTGH-UHFFFAOYSA-N

Formula: C12H10F6O2

SMILES: CC(C)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 300.20

Physical Properties

Property code	Value	Unit	Source
gf	-1256.23	kJ/mol	Joback Method
hf	-1521.66	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	47.18	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.289		Crippen Method
mcvol	174.240	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1153.00		NIST Webbook
tb	575.61	K	Joback Method
tc	756.09	K	Joback Method
tf	342.00	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.59	J/mol×K	575.61	Joback Method
cpg	462.21	J/mol×K	605.69	Joback Method
cpg	474.03	J/mol×K	635.77	Joback Method
cpg	485.09	J/mol×K	665.85	Joback Method
cpg	495.42	J/mol×K	695.93	Joback Method
cpg	505.06	J/mol×K	726.01	Joback Method
cpg	514.05	J/mol×K	756.09	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=U357737&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