2-Fluoro-5-trifluoromethylbenzoic acid, isobutyl ester

Inchi: InChI=1S/C12H12F4O2/c1-7(2)6-18-11(17)9-5-8(12(14,15)16)3-4-10(9)13/h3-5,7H,6H2,1

InchiKey: BIZQLPIQACTQOM-UHFFFAOYSA-N

Formula: C12H12F4O2

SMILES: CC(C)COC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 264.22

Physical Properties

Property code	Value	Unit	Source
gf	-869.45	kJ/mol	Joback Method
hf	-1120.69	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	50.11	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.657		Crippen Method
mcvol	170.700	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	580.30	K	Joback Method
tc	767.10	K	Joback Method
tf	338.40	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.87	J/mol×K	580.30	Joback Method
cpg	442.97	J/mol×K	611.43	Joback Method
cpg	455.32	J/mol×K	642.57	Joback Method
cpg	466.95	J/mol×K	673.70	Joback Method
cpg	477.88	J/mol×K	704.83	Joback Method
cpg	488.14	J/mol×K	735.97	Joback Method
cpg	497.75	J/mol×K	767.10	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=U338956&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