3-Fluoro-4-trifluoromethylbenzoic acid, 3-methylbutyl-2 ester

Inchi: InChI=1S/C13H14F4O2/c1-7(2)8(3)19-12(18)9-4-5-10(11(14)6-9)13(15,16)17/h4-8H,1-3H

InchiKey: FXMKAFZZJLTQQW-UHFFFAOYSA-N

Formula: C13H14F4O2

SMILES: CC(C)C(C)OC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 278.24

Physical Properties

Property code	Value	Unit	Source
gf	-863.47	kJ/mol	Joback Method
hf	-1146.61	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.046		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook
tb	602.74	K	Joback Method
tc	790.95	K	Joback Method
tf	334.67	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.19	J/mol×K	602.74	Joback Method
cpg	493.19	J/mol×K	634.11	Joback Method
cpg	506.37	J/mol×K	665.48	Joback Method
cpg	518.76	J/mol×K	696.84	Joback Method
cpg	530.40	J/mol×K	728.21	Joback Method
cpg	541.32	J/mol×K	759.58	Joback Method
cpg	551.53	J/mol×K	790.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360592&Units=SI

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