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

Inchi: InChI=1S/C14H16F4O3/c1-9(5-6-20-2)8-21-13(19)10-3-4-11(12(15)7-10)14(16,17)18/h3-

InchiKey: XVCPKRAUPVVGTF-UHFFFAOYSA-N

Formula: C14H16F4O3

SMILES: COCCC(C)COC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 308.27

Physical Properties

Property code	Value	Unit	Source
gf	-957.61	kJ/mol	Joback Method
hf	-1294.19	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	56.97	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.674		Crippen Method
mcvol	204.750	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1608.00		NIST Webbook
tb	648.48	K	Joback Method
tc	831.04	K	Joback Method
tf	383.17	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.96	J/mol×K	648.48	Joback Method
cpg	569.91	J/mol×K	678.91	Joback Method
cpg	583.07	J/mol×K	709.33	Joback Method
cpg	595.48	J/mol×K	739.76	Joback Method
cpg	607.16	J/mol×K	770.19	Joback Method
cpg	618.11	J/mol×K	800.61	Joback Method
cpg	628.36	J/mol×K	831.04	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=U360597&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