3-Fluoro-5-trifluoromethylbenzoic acid, 2-methylbutyl ester

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

InchiKey: VCUIIRBHABOYIA-UHFFFAOYSA-N

Formula: C13H14F4O2

SMILES: CCC(C)COC(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 278.24

Physical Properties

Property code	Value	Unit	Source
gf	-861.03	kJ/mol	Joback Method
hf	-1141.33	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.047		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1303.00		NIST Webbook
tb	603.18	K	Joback Method
tc	788.04	K	Joback Method
tf	349.67	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.78	J/mol×K	603.18	Joback Method
cpg	492.48	J/mol×K	633.99	Joback Method
cpg	505.40	J/mol×K	664.80	Joback Method
cpg	517.57	J/mol×K	695.61	Joback Method
cpg	529.02	J/mol×K	726.42	Joback Method
cpg	539.78	J/mol×K	757.23	Joback Method
cpg	549.87	J/mol×K	788.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357340&Units=SI
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

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

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