3-Methoxy-2,4,5-trifluorobenzoic acid, 3-methylbutyl-2 ester

Inchi: InChI=1S/C13H15F3O3/c1-6(2)7(3)19-13(17)8-5-9(14)11(16)12(18-4)10(8)15/h5-7H,1-4

InchiKey: FYPUOUBIXLJJJI-UHFFFAOYSA-N

Formula: C13H15F3O3

SMILES: COc1c(F)c(F)cc(C(=O)OC(C)C(C)C)c1F

Mol. weight [g/mol]: 276.25

Physical Properties

Property code	Value	Unit	Source
gf	-795.76	kJ/mol	Joback Method
hf	-1096.91	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.314		Crippen Method
mcvol	188.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	639.08	K	Joback Method
tc	826.49	K	Joback Method
tf	378.93	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.87	J/mol×K	639.08	Joback Method
cpg	506.29	J/mol×K	670.31	Joback Method
cpg	519.07	J/mol×K	701.55	Joback Method
cpg	531.20	J/mol×K	732.78	Joback Method
cpg	542.67	J/mol×K	764.02	Joback Method
cpg	553.49	J/mol×K	795.25	Joback Method
cpg	563.64	J/mol×K	826.49	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=U360568&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