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

Inchi: InChI=1S/C13H15F3O3/c1-7(2)4-5-19-13(17)8-6-9(14)11(16)12(18-3)10(8)15/h6-7H,4-5
InchiKey: JYPKDBYMJHSICM-UHFFFAOYSA-N
Formula: C13H15F3O3
SMILES: COc1c(F)c(F)cc(C(=O)OCCC(C)C)c1F
Mol. weight [g/mol]: 276.25

Physical Properties

Property code	Value	Unit	Source
gf	-793.32	kJ/mol	Joback Method
hf	-1091.63	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.315		Crippen Method
mcvol	188.890	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1606.00		NIST Webbook
tb	639.52	K	Joback Method
tc	823.86	K	Joback Method
tf	393.93	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.40	J/mol×K	639.52	Joback Method
cpg	505.56	J/mol×K	670.24	Joback Method
cpg	518.11	J/mol×K	700.97	Joback Method
cpg	530.04	J/mol×K	731.69	Joback Method
cpg	541.35	J/mol×K	762.42	Joback Method
cpg	552.03	J/mol×K	793.14	Joback Method
cpg	562.07	J/mol×K	823.86	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=U360569&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