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

Inchi: InChI=1S/C12H13F3O3/c1-6(2)5-18-12(16)7-4-8(13)10(15)11(17-3)9(7)14/h4,6H,5H2,1-3

InchiKey: MZRXTTMFOIURDO-UHFFFAOYSA-N

Formula: C12H13F3O3

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

Mol. weight [g/mol]: 262.23

Physical Properties

Property code	Value	Unit	Source
gf	-801.74	kJ/mol	Joback Method
hf	-1070.99	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.925		Crippen Method
mcvol	174.800	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	616.64	K	Joback Method
tc	802.63	K	Joback Method
tf	382.66	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.43	J/mol×K	616.64	Joback Method
cpg	454.91	J/mol×K	647.64	Joback Method
cpg	466.83	J/mol×K	678.64	Joback Method
cpg	478.18	J/mol×K	709.64	Joback Method
cpg	488.95	J/mol×K	740.63	Joback Method
cpg	499.15	J/mol×K	771.63	Joback Method
cpg	508.75	J/mol×K	802.63	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=U338759&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