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

Inchi: InChI=1S/C10H9F3O3/c1-3-16-10(14)5-4-6(11)8(13)9(15-2)7(5)12/h4H,3H2,1-2H3
InchiKey: ZXFYRSUEOKXKOQ-UHFFFAOYSA-N
Formula: C10H9F3O3
SMILES: CCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 234.17

Physical Properties

Property code	Value	Unit	Source
gf	-816.14	kJ/mol	Joback Method
hf	-1024.43	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.289		Crippen Method
mcvol	146.620	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1334.00		NIST Webbook
tb	571.32	K	Joback Method
tc	757.81	K	Joback Method
tf	375.12	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.98	J/mol×K	571.32	Joback Method
cpg	357.54	J/mol×K	602.40	Joback Method
cpg	367.69	J/mol×K	633.48	Joback Method
cpg	377.41	J/mol×K	664.57	Joback Method
cpg	386.69	J/mol×K	695.65	Joback Method
cpg	395.52	J/mol×K	726.73	Joback Method
cpg	403.88	J/mol×K	757.81	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=U338757&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