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

Inchi: InChI=1S/C11H11F3O3/c1-3-4-17-11(15)6-5-7(12)9(14)10(16-2)8(6)13/h5H,3-4H2,1-2H3

InchiKey: XTSVIRJJHPVMEP-UHFFFAOYSA-N

Formula: C11H11F3O3

SMILES: CCCOC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 248.20

Physical Properties

Property code	Value	Unit	Source
gf	-807.72	kJ/mol	Joback Method
hf	-1045.07	kJ/mol	Joback Method
hfus	29.95	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.679		Crippen Method
mcvol	160.710	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
tb	594.20	K	Joback Method
tc	778.74	K	Joback Method
tf	386.39	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.62	J/mol×K	594.20	Joback Method
cpg	405.07	J/mol×K	624.96	Joback Method
cpg	416.03	J/mol×K	655.71	Joback Method
cpg	426.52	J/mol×K	686.47	Joback Method
cpg	436.50	J/mol×K	717.23	Joback Method
cpg	445.98	J/mol×K	747.98	Joback Method
cpg	454.95	J/mol×K	778.74	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=U338758&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