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

Inchi: InChI=1S/C17H15F3O3/c1-3-6-10-7-4-5-8-13(10)23-17(21)11-9-12(18)15(20)16(22-2)14

InchiKey: PFPKVRQSXIDVMQ-UHFFFAOYSA-N

Formula: C17H15F3O3

SMILES: CCCc1ccccc1OC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 324.29

Physical Properties

Property code	Value	Unit	Source
gf	-654.42	kJ/mol	Joback Method
hf	-943.85	kJ/mol	Joback Method
hfus	39.14	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.284		Crippen Method
mcvol	221.490	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	763.14	K	Joback Method
tc	968.78	K	Joback Method
tf	492.95	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.56	J/mol×K	763.14	Joback Method
cpg	630.99	J/mol×K	797.41	Joback Method
cpg	643.48	J/mol×K	831.69	Joback Method
cpg	655.04	J/mol×K	865.96	Joback Method
cpg	665.67	J/mol×K	900.23	Joback Method
cpg	675.37	J/mol×K	934.50	Joback Method
cpg	684.15	J/mol×K	968.78	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=U360573&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