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

Inchi: InChI=1S/C19H27F3O3/c1-3-4-5-6-7-8-9-10-11-12-25-19(23)14-13-15(20)17(22)18(24-2
InchiKey: YUSVYGSZQZGROO-UHFFFAOYSA-N
Formula: C19H27F3O3
SMILES: CCCCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 360.41

Physical Properties

Property code	Value	Unit	Source
gf	-740.36	kJ/mol	Joback Method
hf	-1210.19	kJ/mol	Joback Method
hfus	50.67	kJ/mol	Joback Method
hvap	71.93	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.800		Crippen Method
mcvol	273.430	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2251.00		NIST Webbook
rinpol	2251.00		NIST Webbook
tb	777.24	K	Joback Method
tc	959.21	K	Joback Method
tf	476.55	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.75	J/mol×K	777.24	Joback Method
cpg	835.67	J/mol×K	807.57	Joback Method
cpg	850.70	J/mol×K	837.90	Joback Method
cpg	864.84	J/mol×K	868.22	Joback Method
cpg	878.09	J/mol×K	898.55	Joback Method
cpg	890.47	J/mol×K	928.88	Joback Method
cpg	901.98	J/mol×K	959.21	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=U338768&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