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

Inchi: InChI=1S/C17H23F3O3/c1-3-4-5-6-7-8-9-10-23-17(21)12-11-13(18)15(20)16(22-2)14(12
InchiKey: SNMQVKPKVOMNJR-UHFFFAOYSA-N
Formula: C17H23F3O3
SMILES: CCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 332.36

Physical Properties

Property code	Value	Unit	Source
gf	-757.20	kJ/mol	Joback Method
hf	-1168.91	kJ/mol	Joback Method
hfus	45.49	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.020		Crippen Method
mcvol	245.250	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	731.48	K	Joback Method
tc	911.20	K	Joback Method
tf	454.01	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.75	J/mol×K	731.48	Joback Method
cpg	720.81	J/mol×K	761.43	Joback Method
cpg	735.09	J/mol×K	791.39	Joback Method
cpg	748.58	J/mol×K	821.34	Joback Method
cpg	761.29	J/mol×K	851.29	Joback Method
cpg	773.22	J/mol×K	881.25	Joback Method
cpg	784.38	J/mol×K	911.20	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=U338766&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