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

Inchi: InChI=1S/C27H43F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-33-27(31)2
InchiKey: ADARQHFTLBMETO-UHFFFAOYSA-N
Formula: C27H43F3O3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 472.62

Physical Properties

Property code	Value	Unit	Source
gf	-673.00	kJ/mol	Joback Method
hf	-1375.31	kJ/mol	Joback Method
hfus	71.39	kJ/mol	Joback Method
hvap	89.73	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.921		Crippen Method
mcvol	386.150	ml/mol	McGowan Method
pc	752.67	kPa	Joback Method
rinpol	3070.00		NIST Webbook
rinpol	3070.00		NIST Webbook
tb	960.28	K	Joback Method
tc	1182.85	K	Joback Method
tf	566.71	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.90	J/mol×K	960.28	Joback Method
cpg	1327.51	J/mol×K	997.37	Joback Method
cpg	1345.42	J/mol×K	1034.47	Joback Method
cpg	1361.68	J/mol×K	1071.56	Joback Method
cpg	1376.33	J/mol×K	1108.66	Joback Method
cpg	1389.42	J/mol×K	1145.75	Joback Method
cpg	1400.97	J/mol×K	1182.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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