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

Inchi: InChI=1S/C21H31F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-27-21(25)16-15-17(22)19(24)2

InchiKey: LKLGHQDMQLRCGZ-UHFFFAOYSA-N

Formula: C21H31F3O3

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

Mol. weight [g/mol]: 388.46

Physical Properties

Property code	Value	Unit	Source
gf	-723.52	kJ/mol	Joback Method
hf	-1251.47	kJ/mol	Joback Method
hfus	55.85	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.580		Crippen Method
mcvol	301.610	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	823.00	K	Joback Method
tc	1009.86	K	Joback Method
tf	499.09	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.55	J/mol×K	823.00	Joback Method
cpg	954.31	J/mol×K	854.14	Joback Method
cpg	970.03	J/mol×K	885.29	Joback Method
cpg	984.74	J/mol×K	916.43	Joback Method
cpg	998.45	J/mol×K	947.57	Joback Method
cpg	1011.16	J/mol×K	978.72	Joback Method
cpg	1022.89	J/mol×K	1009.86	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=U338770&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