2,4,5-Trifluoro-3-methoxybenzoic acid, 5-tridecyl ester

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

InchiKey: SFOBYSWKHYZLLV-UHFFFAOYSA-N

Formula: C21H31F3O3

SMILES: CCCCCCCCC(CCCC)OC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 388.46

Physical Properties

Property code	Value	Unit	Source
gf	-725.96	kJ/mol	Joback Method
hf	-1256.75	kJ/mol	Joback Method
hfus	52.32	kJ/mol	Joback Method
hvap	75.99	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.579		Crippen Method
mcvol	301.610	ml/mol	McGowan Method
pc	1067.27	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	822.56	K	Joback Method
tc	1010.16	K	Joback Method
tf	484.09	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.05	J/mol×K	822.56	Joback Method
cpg	954.87	J/mol×K	853.83	Joback Method
cpg	970.64	J/mol×K	885.09	Joback Method
cpg	985.38	J/mol×K	916.36	Joback Method
cpg	999.10	J/mol×K	947.63	Joback Method
cpg	1011.81	J/mol×K	978.89	Joback Method
cpg	1023.52	J/mol×K	1010.16	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=U338459&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