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

Inchi: InChI=1S/C22H33F3O3/c1-4-5-6-7-8-9-10-11-12-13-14-16(2)28-22(26)17-15-18(23)20(2

InchiKey: SHZDZHHNHYUNIK-UHFFFAOYSA-N

Formula: C22H33F3O3

SMILES: CCCCCCCCCCCCC(C)OC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 402.49

Physical Properties

Property code	Value	Unit	Source
gf	-717.54	kJ/mol	Joback Method
hf	-1277.39	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.969		Crippen Method
mcvol	315.700	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	845.44	K	Joback Method
tc	1036.30	K	Joback Method
tf	495.36	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/mol×K	845.44	Joback Method
cpg	1015.38	J/mol×K	877.25	Joback Method
cpg	1031.47	J/mol×K	909.06	Joback Method
cpg	1046.45	J/mol×K	940.87	Joback Method
cpg	1060.34	J/mol×K	972.68	Joback Method
cpg	1073.15	J/mol×K	1004.49	Joback Method
cpg	1084.91	J/mol×K	1036.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338461&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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