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

Inchi: InChI=1S/C23H35F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-29-23(27)18-17-19(24)2

InchiKey: YCZAUIKJMXBMLS-UHFFFAOYSA-N

Formula: C23H35F3O3

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

Mol. weight [g/mol]: 416.52

Physical Properties

Property code	Value	Unit	Source
gf	-706.68	kJ/mol	Joback Method
hf	-1292.75	kJ/mol	Joback Method
hfus	61.03	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.361		Crippen Method
mcvol	329.790	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	868.76	K	Joback Method
tc	1063.64	K	Joback Method
tf	521.63	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.55	J/mol×K	868.76	Joback Method
cpg	1076.16	J/mol×K	901.24	Joback Method
cpg	1092.58	J/mol×K	933.72	Joback Method
cpg	1107.83	J/mol×K	966.20	Joback Method
cpg	1121.92	J/mol×K	998.68	Joback Method
cpg	1134.87	J/mol×K	1031.16	Joback Method
cpg	1146.70	J/mol×K	1063.64	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=U338772&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