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

Inchi: InChI=1S/C24H37F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-30-24(28)19-18-20(2

InchiKey: BEWHNOHENBEDJQ-UHFFFAOYSA-N

Formula: C24H37F3O3

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

Mol. weight [g/mol]: 430.54

Physical Properties

Property code	Value	Unit	Source
gf	-698.26	kJ/mol	Joback Method
hf	-1313.39	kJ/mol	Joback Method
hfus	63.62	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.751		Crippen Method
mcvol	343.880	ml/mol	McGowan Method
pc	887.35	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
tb	891.64	K	Joback Method
tc	1091.87	K	Joback Method
tf	532.90	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.06	J/mol×K	891.64	Joback Method
cpg	1138.13	J/mol×K	925.01	Joback Method
cpg	1154.91	J/mol×K	958.38	Joback Method
cpg	1170.42	J/mol×K	991.76	Joback Method
cpg	1184.68	J/mol×K	1025.13	Joback Method
cpg	1197.71	J/mol×K	1058.50	Joback Method
cpg	1209.54	J/mol×K	1091.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338773&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