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

Inchi: InChI=1S/C26H41F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-32-26(30)21-2
InchiKey: VKCXXFKERXCBOZ-UHFFFAOYSA-N
Formula: C26H41F3O3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 458.60

Physical Properties

Property code	Value	Unit	Source
gf	-681.42	kJ/mol	Joback Method
hf	-1354.67	kJ/mol	Joback Method
hfus	68.80	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.531		Crippen Method
mcvol	372.060	ml/mol	McGowan Method
pc	793.94	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	937.40	K	Joback Method
tc	1151.39	K	Joback Method
tf	555.44	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.80	J/mol×K	937.40	Joback Method
cpg	1263.86	J/mol×K	973.07	Joback Method
cpg	1281.39	J/mol×K	1008.73	Joback Method
cpg	1297.40	J/mol×K	1044.40	Joback Method
cpg	1311.95	J/mol×K	1080.06	Joback Method
cpg	1325.05	J/mol×K	1115.73	Joback Method
cpg	1336.75	J/mol×K	1151.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338775&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

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