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

Inchi: InChI=1S/C25H39F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-31-25(29)20-19-2

InchiKey: KZZLAHHYIWSXAB-UHFFFAOYSA-N

Formula: C25H39F3O3

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

Mol. weight [g/mol]: 444.57

Physical Properties

Property code	Value	Unit	Source
gf	-689.84	kJ/mol	Joback Method
hf	-1334.03	kJ/mol	Joback Method
hfus	66.21	kJ/mol	Joback Method
hvap	85.28	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.141		Crippen Method
mcvol	357.970	ml/mol	McGowan Method
pc	838.70	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	914.52	K	Joback Method
tc	1121.10	K	Joback Method
tf	544.17	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.17	J/mol×K	914.52	Joback Method
cpg	1200.72	J/mol×K	948.95	Joback Method
cpg	1217.86	J/mol×K	983.38	Joback Method
cpg	1233.63	J/mol×K	1017.81	Joback Method
cpg	1248.04	J/mol×K	1052.24	Joback Method
cpg	1261.13	J/mol×K	1086.67	Joback Method
cpg	1272.91	J/mol×K	1121.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338774&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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