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

Inchi: InChI=1S/C16H21F3O3/c1-3-4-5-6-7-8-9-22-16(20)11-10-12(17)14(19)15(21-2)13(11)18

InchiKey: GLWASYKJMDNIHJ-UHFFFAOYSA-N

Formula: C16H21F3O3

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

Mol. weight [g/mol]: 318.33

Physical Properties

Property code	Value	Unit	Source
gf	-765.62	kJ/mol	Joback Method
hf	-1148.27	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.630		Crippen Method
mcvol	231.160	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	708.60	K	Joback Method
tc	888.05	K	Joback Method
tf	442.74	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.39	J/mol×K	708.60	Joback Method
cpg	664.98	J/mol×K	738.51	Joback Method
cpg	678.84	J/mol×K	768.42	Joback Method
cpg	691.97	J/mol×K	798.33	Joback Method
cpg	704.36	J/mol×K	828.23	Joback Method
cpg	716.01	J/mol×K	858.14	Joback Method
cpg	726.94	J/mol×K	888.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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