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

Inchi: InChI=1S/C13H15F3O3/c1-3-4-5-6-19-13(17)8-7-9(14)11(16)12(18-2)10(8)15/h7H,3-6H2

InchiKey: OGTBZRYVGJYGGC-UHFFFAOYSA-N

Formula: C13H15F3O3

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

Mol. weight [g/mol]: 276.25

Physical Properties

Property code	Value	Unit	Source
gf	-790.88	kJ/mol	Joback Method
hf	-1086.35	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.460		Crippen Method
mcvol	188.890	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	639.96	K	Joback Method
tc	821.38	K	Joback Method
tf	408.93	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.93	J/mol×K	639.96	Joback Method
cpg	504.85	J/mol×K	670.20	Joback Method
cpg	517.18	J/mol×K	700.43	Joback Method
cpg	528.92	J/mol×K	730.67	Joback Method
cpg	540.06	J/mol×K	760.90	Joback Method
cpg	550.60	J/mol×K	791.14	Joback Method
cpg	560.54	J/mol×K	821.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338761&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