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

Inchi: InChI=1S/C14H17F3O3/c1-8(2)5-4-6-20-14(18)9-7-10(15)12(17)13(19-3)11(9)16/h7-8H,4

InchiKey: MSFTVYVSPAYJIU-UHFFFAOYSA-N

Formula: C14H17F3O3

SMILES: COc1c(F)c(F)cc(C(=O)OCCCC(C)C)c1F

Mol. weight [g/mol]: 290.28

Physical Properties

Property code	Value	Unit	Source
gf	-784.90	kJ/mol	Joback Method
hf	-1112.27	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.706		Crippen Method
mcvol	202.980	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	662.40	K	Joback Method
tc	845.44	K	Joback Method
tf	405.20	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.87	J/mol×K	662.40	Joback Method
cpg	557.64	J/mol×K	692.91	Joback Method
cpg	570.74	J/mol×K	723.41	Joback Method
cpg	583.18	J/mol×K	753.92	Joback Method
cpg	594.94	J/mol×K	784.42	Joback Method
cpg	606.04	J/mol×K	814.93	Joback Method
cpg	616.45	J/mol×K	845.44	Joback Method

Sources

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=U338762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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