2,4,5-Trifluoro-3-methoxybenzoic acid, methyl ester

Inchi: InChI=1S/C9H7F3O3/c1-14-8-6(11)4(9(13)15-2)3-5(10)7(8)12/h3H,1-2H3
InchiKey: WRNVSUJHRFXTKQ-UHFFFAOYSA-N
Formula: C9H7F3O3
SMILES: COC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 220.15

Physical Properties

Property code	Value	Unit	Source
gf	-824.56	kJ/mol	Joback Method
hf	-1003.79	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.899		Crippen Method
mcvol	132.530	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1262.00		NIST Webbook
tb	548.44	K	Joback Method
tc	737.08	K	Joback Method
tf	363.85	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.15	J/mol×K	548.44	Joback Method
cpg	311.72	J/mol×K	579.88	Joback Method
cpg	320.94	J/mol×K	611.32	Joback Method
cpg	329.80	J/mol×K	642.76	Joback Method
cpg	338.28	J/mol×K	674.20	Joback Method
cpg	346.36	J/mol×K	705.64	Joback Method
cpg	354.03	J/mol×K	737.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357622&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