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

Inchi: InChI=1S/C12H13F3O3/c1-3-4-5-18-12(16)7-6-8(13)10(15)11(17-2)9(7)14/h6H,3-5H2,1-

InchiKey: ZDFCVSGBTYDIFV-UHFFFAOYSA-N

Formula: C12H13F3O3

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

Mol. weight [g/mol]: 262.23

Physical Properties

Property code	Value	Unit	Source
gf	-799.30	kJ/mol	Joback Method
hf	-1065.71	kJ/mol	Joback Method
hfus	32.54	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.069		Crippen Method
mcvol	174.800	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	617.08	K	Joback Method
tc	799.91	K	Joback Method
tf	397.66	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.98	J/mol×K	617.08	Joback Method
cpg	454.20	J/mol×K	647.55	Joback Method
cpg	465.89	J/mol×K	678.02	Joback Method
cpg	477.04	J/mol×K	708.49	Joback Method
cpg	487.65	J/mol×K	738.97	Joback Method
cpg	497.69	J/mol×K	769.44	Joback Method
cpg	507.18	J/mol×K	799.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338760&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