3-Methoxy-2,4,5-trifluorobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H5Cl4F3O3/c1-23-13-10(20)4(2-7(19)11(13)21)14(22)24-12-6(16)3-5(15)8

InchiKey: KOOVJMJUKYVOGD-UHFFFAOYSA-N

Formula: C14H5Cl4F3O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2c(Cl)cc(Cl)c(Cl)c2Cl)c1F

Mol. weight [g/mol]: 420.00

Physical Properties

Property code	Value	Unit	Source
gf	-756.29	kJ/mol	Joback Method
hf	-979.30	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	83.26	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	5.945		Crippen Method
mcvol	228.180	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	859.16	K	Joback Method
tc	1086.82	K	Joback Method
tf	616.38	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.65	J/mol×K	859.16	Joback Method
cpg	544.32	J/mol×K	897.10	Joback Method
cpg	551.09	J/mol×K	935.05	Joback Method
cpg	556.94	J/mol×K	972.99	Joback Method
cpg	561.86	J/mol×K	1010.93	Joback Method
cpg	565.82	J/mol×K	1048.87	Joback Method
cpg	568.81	J/mol×K	1086.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360576&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