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

Inchi: InChI=1S/C14H6Cl3F3O3/c1-22-13-11(19)5(2-9(18)12(13)20)14(21)23-10-4-7(16)6(15)3

InchiKey: XJURORRGGKGZNA-UHFFFAOYSA-N

Formula: C14H6Cl3F3O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)c1F

Mol. weight [g/mol]: 385.55

Physical Properties

Property code	Value	Unit	Source
gf	-734.73	kJ/mol	Joback Method
hf	-952.09	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	78.21	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.292		Crippen Method
mcvol	215.940	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	816.75	K	Joback Method
tc	1040.61	K	Joback Method
tf	573.94	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.44	J/mol×K	816.75	Joback Method
cpg	529.25	J/mol×K	854.06	Joback Method
cpg	537.20	J/mol×K	891.37	Joback Method
cpg	544.28	J/mol×K	928.68	Joback Method
cpg	550.46	J/mol×K	965.99	Joback Method
cpg	555.74	J/mol×K	1003.30	Joback Method
cpg	560.10	J/mol×K	1040.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360575&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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