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

Inchi: InChI=1S/C14H7Cl2F3O3/c1-21-13-11(18)7(5-10(17)12(13)19)14(20)22-6-2-3-8(15)9(16
InchiKey: QMWUERZZEODEIV-UHFFFAOYSA-N
Formula: C14H7Cl2F3O3
SMILES: COc1c(F)c(F)cc(C(=O)Oc2ccc(Cl)c(Cl)c2)c1F
Mol. weight [g/mol]: 351.11

Physical Properties

Property code	Value	Unit	Source
gf	-713.17	kJ/mol	Joback Method
hf	-924.88	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.639		Crippen Method
mcvol	203.700	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	774.34	K	Joback Method
tc	994.45	K	Joback Method
tf	531.50	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.43	J/mol×K	774.34	Joback Method
cpg	512.37	J/mol×K	811.02	Joback Method
cpg	521.47	J/mol×K	847.71	Joback Method
cpg	529.72	J/mol×K	884.39	Joback Method
cpg	537.11	J/mol×K	921.08	Joback Method
cpg	543.64	J/mol×K	957.76	Joback Method
cpg	549.30	J/mol×K	994.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357619&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