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

Inchi: InChI=1S/C14H8ClF3O3/c1-20-13-11(17)9(6-10(16)12(13)18)14(19)21-8-4-2-7(15)3-5-8/

InchiKey: KWOJHFPOKLTYKN-UHFFFAOYSA-N

Formula: C14H8ClF3O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2ccc(Cl)cc2)c1F

Mol. weight [g/mol]: 316.66

Physical Properties

Property code	Value	Unit	Source
gf	-691.61	kJ/mol	Joback Method
hf	-897.67	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.985		Crippen Method
mcvol	191.460	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2033.00		NIST Webbook
tb	731.93	K	Joback Method
tc	948.21	K	Joback Method
tf	489.06	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.52	J/mol×K	731.93	Joback Method
cpg	493.59	J/mol×K	767.98	Joback Method
cpg	503.83	J/mol×K	804.02	Joback Method
cpg	513.24	J/mol×K	840.07	Joback Method
cpg	521.81	J/mol×K	876.12	Joback Method
cpg	529.54	J/mol×K	912.17	Joback Method
cpg	536.43	J/mol×K	948.21	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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