2,3,4-Trifluorobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H5Cl2F3O2/c14-8-3-1-6(5-9(8)15)20-13(19)7-2-4-10(16)12(18)11(7)17/h1-

InchiKey: UKUPWIAAVFOYPQ-UHFFFAOYSA-N

Formula: C13H5Cl2F3O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 321.08

Physical Properties

Property code	Value	Unit	Source
gf	-606.96	kJ/mol	Joback Method
hf	-760.55	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	67.87	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.630		Crippen Method
mcvol	183.740	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
tb	724.06	K	Joback Method
tc	949.16	K	Joback Method
tf	485.48	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.51	J/mol×K	724.06	Joback Method
cpg	439.20	J/mol×K	761.58	Joback Method
cpg	448.10	J/mol×K	799.09	Joback Method
cpg	456.23	J/mol×K	836.61	Joback Method
cpg	463.61	J/mol×K	874.13	Joback Method
cpg	470.25	J/mol×K	911.64	Joback Method
cpg	476.16	J/mol×K	949.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308035&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