3-Fluoro-4-trifluoromethylbenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H5Cl3F4O2/c15-8-4-10(17)12(5-9(8)16)23-13(22)6-1-2-7(11(18)3-6)14(19,

InchiKey: KKORITHVGLTYGK-UHFFFAOYSA-N

Formula: C14H5Cl3F4O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 387.54

Physical Properties

Property code	Value	Unit	Source
gf	-802.44	kJ/mol	Joback Method
hf	-1001.79	kJ/mol	Joback Method
hfus	38.44	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.024		Crippen Method
mcvol	211.840	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2092.00		NIST Webbook
tb	780.41	K	Joback Method
tc	1006.73	K	Joback Method
tf	529.68	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.79	J/mol×K	780.41	Joback Method
cpg	519.63	J/mol×K	818.13	Joback Method
cpg	527.65	J/mol×K	855.85	Joback Method
cpg	534.88	J/mol×K	893.57	Joback Method
cpg	541.37	J/mol×K	931.29	Joback Method
cpg	547.16	J/mol×K	969.01	Joback Method
cpg	552.30	J/mol×K	1006.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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