3-Fluoro-4-trifluoromethylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H4Cl4F4O2/c15-7-4-8(16)12(11(18)10(7)17)24-13(23)5-1-2-6(9(19)3-5)14(

InchiKey: IDXBKJIJQFAJBD-UHFFFAOYSA-N

Formula: C14H4Cl4F4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 421.99

Physical Properties

Property code	Value	Unit	Source
gf	-824.00	kJ/mol	Joback Method
hf	-1029.00	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.677		Crippen Method
mcvol	224.080	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	822.82	K	Joback Method
tc	1052.62	K	Joback Method
tf	572.12	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.22	J/mol×K	822.82	Joback Method
cpg	534.94	J/mol×K	861.12	Joback Method
cpg	541.88	J/mol×K	899.42	Joback Method
cpg	548.07	J/mol×K	937.72	Joback Method
cpg	553.56	J/mol×K	976.02	Joback Method
cpg	558.39	J/mol×K	1014.32	Joback Method
cpg	562.60	J/mol×K	1052.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360601&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

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