3-Trifluoromethylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H5Cl4F3O2/c15-8-5-9(16)12(11(18)10(8)17)23-13(22)6-2-1-3-7(4-6)14(19,

InchiKey: NTTDMPDJMIPWJH-UHFFFAOYSA-N

Formula: C14H5Cl4F3O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 404.00

Physical Properties

Property code	Value	Unit	Source
gf	-619.56	kJ/mol	Joback Method
hf	-821.42	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	77.57	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.538		Crippen Method
mcvol	222.310	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	818.57	K	Joback Method
tc	1056.29	K	Joback Method
tf	559.01	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.62	J/mol×K	818.57	Joback Method
cpg	529.83	J/mol×K	858.19	Joback Method
cpg	537.19	J/mol×K	897.81	Joback Method
cpg	543.75	J/mol×K	937.43	Joback Method
cpg	549.58	J/mol×K	977.05	Joback Method
cpg	554.71	J/mol×K	1016.67	Joback Method
cpg	559.21	J/mol×K	1056.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355146&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