3-Trifluoromethylbenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H6Cl3F3O2/c15-9-5-11(17)12(6-10(9)16)22-13(21)7-2-1-3-8(4-7)14(18,19)

InchiKey: GGVWPJANJLZFBO-UHFFFAOYSA-N

Formula: C14H6Cl3F3O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 369.55

Physical Properties

Property code	Value	Unit	Source
gf	-598.00	kJ/mol	Joback Method
hf	-794.21	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	72.52	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.885		Crippen Method
mcvol	210.070	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	776.16	K	Joback Method
tc	1010.79	K	Joback Method
tf	516.57	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.89	J/mol×K	776.16	Joback Method
cpg	514.29	J/mol×K	815.26	Joback Method
cpg	522.78	J/mol×K	854.37	Joback Method
cpg	530.43	J/mol×K	893.47	Joback Method
cpg	537.28	J/mol×K	932.58	Joback Method
cpg	543.40	J/mol×K	971.68	Joback Method
cpg	548.84	J/mol×K	1010.79	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=U355145&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