3-Trifluoromethylbenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H7Cl2F3O2/c15-11-5-4-10(7-12(11)16)21-13(20)8-2-1-3-9(6-8)14(17,18)19

InchiKey: XEPBLASLHWVJHK-UHFFFAOYSA-N

Formula: C14H7Cl2F3O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 335.11

Physical Properties

Property code	Value	Unit	Source
gf	-576.44	kJ/mol	Joback Method
hf	-767.00	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	67.47	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.231		Crippen Method
mcvol	197.830	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	733.75	K	Joback Method
tc	965.13	K	Joback Method
tf	474.13	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.25	J/mol×K	733.75	Joback Method
cpg	496.93	J/mol×K	772.31	Joback Method
cpg	506.63	J/mol×K	810.88	Joback Method
cpg	515.43	J/mol×K	849.44	Joback Method
cpg	523.37	J/mol×K	888.01	Joback Method
cpg	530.52	J/mol×K	926.57	Joback Method
cpg	536.94	J/mol×K	965.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307681&Units=SI

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