4-Trifluoromethylbenzoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H8ClF3O2/c15-11-5-7-12(8-6-11)20-13(19)9-1-3-10(4-2-9)14(16,17)18/h1-

InchiKey: STHLRRJMXBVNPV-UHFFFAOYSA-N

Formula: C14H8ClF3O2

SMILES: O=C(Oc1ccc(Cl)cc1)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 300.66

Physical Properties

Property code	Value	Unit	Source
gf	-554.88	kJ/mol	Joback Method
hf	-739.79	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.578		Crippen Method
mcvol	185.590	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	691.34	K	Joback Method
tc	919.23	K	Joback Method
tf	431.69	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.51	J/mol×K	691.34	Joback Method
cpg	477.56	J/mol×K	729.32	Joback Method
cpg	488.56	J/mol×K	767.30	Joback Method
cpg	498.59	J/mol×K	805.28	Joback Method
cpg	507.70	J/mol×K	843.27	Joback Method
cpg	515.95	J/mol×K	881.25	Joback Method
cpg	523.41	J/mol×K	919.23	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=U307734&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