2,3,4-Trifluorobenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H9F3O2/c1-8-3-2-4-9(7-8)19-14(18)10-5-6-11(15)13(17)12(10)16/h2-7H,1
InchiKey: DCACKVNSSVKRSY-UHFFFAOYSA-N
Formula: C14H9F3O2
SMILES: Cc1cccc(OC(=O)c2ccc(F)c(F)c2F)c1
Mol. weight [g/mol]: 266.22

Physical Properties

Property code	Value	Unit	Source
gf	-565.05	kJ/mol	Joback Method
hf	-738.24	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.632		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1693.00		NIST Webbook
tb	667.10	K	Joback Method
tc	881.67	K	Joback Method
tf	424.39	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.00	J/mol×K	667.10	Joback Method
cpg	448.44	J/mol×K	702.86	Joback Method
cpg	460.05	J/mol×K	738.62	Joback Method
cpg	470.83	J/mol×K	774.38	Joback Method
cpg	480.82	J/mol×K	810.15	Joback Method
cpg	490.03	J/mol×K	845.91	Joback Method
cpg	498.46	J/mol×K	881.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308030&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