2,4,5-Trifluoro-3-methoxybenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H11F3O3/c1-8-4-3-5-9(6-8)21-15(19)10-7-11(16)13(18)14(20-2)12(10)17/h

InchiKey: CMTRCIXUUHEUFD-UHFFFAOYSA-N

Formula: C15H11F3O3

SMILES: COc1c(F)c(F)cc(C(=O)Oc2cccc(C)c2)c1F

Mol. weight [g/mol]: 296.24

Physical Properties

Property code	Value	Unit	Source
gf	-671.26	kJ/mol	Joback Method
hf	-902.57	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	65.96	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.640		Crippen Method
mcvol	193.310	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	717.38	K	Joback Method
tc	927.55	K	Joback Method
tf	470.41	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.88	J/mol×K	717.38	Joback Method
cpg	523.48	J/mol×K	752.41	Joback Method
cpg	535.22	J/mol×K	787.44	Joback Method
cpg	546.12	J/mol×K	822.46	Joback Method
cpg	556.16	J/mol×K	857.49	Joback Method
cpg	565.34	J/mol×K	892.52	Joback Method
cpg	573.67	J/mol×K	927.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357614&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