2,3,4-Trifluorobenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H11F3O2/c1-8-5-9(2)7-10(6-8)20-15(19)11-3-4-12(16)14(18)13(11)17/h3-7

InchiKey: JFBJHQAKRZWJKB-UHFFFAOYSA-N

Formula: C15H11F3O2

SMILES: Cc1cc(C)cc(OC(=O)c2ccc(F)c(F)c2F)c1

Mol. weight [g/mol]: 280.24

Physical Properties

Property code	Value	Unit	Source
gf	-566.26	kJ/mol	Joback Method
hf	-770.35	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	3.940		Crippen Method
mcvol	187.440	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	694.96	K	Joback Method
tc	907.10	K	Joback Method
tf	448.18	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.58	J/mol×K	694.96	Joback Method
cpg	498.43	J/mol×K	730.32	Joback Method
cpg	510.44	J/mol×K	765.67	Joback Method
cpg	521.62	J/mol×K	801.03	Joback Method
cpg	531.98	J/mol×K	836.38	Joback Method
cpg	541.54	J/mol×K	871.74	Joback Method
cpg	550.31	J/mol×K	907.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308032&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

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