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

Inchi: InChI=1S/C15H11F3O4/c1-20-8-3-5-9(6-4-8)22-15(19)10-7-11(16)13(18)14(21-2)12(10)1

InchiKey: XUOVIFLADDYXCT-UHFFFAOYSA-N

Formula: C15H11F3O4

SMILES: COc1ccc(OC(=O)c2cc(F)c(F)c(OC)c2F)cc1

Mol. weight [g/mol]: 312.24

Physical Properties

Property code	Value	Unit	Source
gf	-776.26	kJ/mol	Joback Method
hf	-1034.79	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	68.37	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.340		Crippen Method
mcvol	199.180	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	739.80	K	Joback Method
tc	948.30	K	Joback Method
tf	492.64	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.35	J/mol×K	739.80	Joback Method
cpg	548.68	J/mol×K	774.55	Joback Method
cpg	560.13	J/mol×K	809.30	Joback Method
cpg	570.69	J/mol×K	844.05	Joback Method
cpg	580.34	J/mol×K	878.80	Joback Method
cpg	589.07	J/mol×K	913.55	Joback Method
cpg	596.86	J/mol×K	948.30	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=U357617&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