2,6-Dimethoxyphenol, trifluoroacetate

Inchi: InChI=1S/C10H9F3O4/c1-15-6-4-3-5-7(16-2)8(6)17-9(14)10(11,12)13/h3-5H,1-2H3
InchiKey: LPPURHYBXVOBFD-UHFFFAOYSA-N
Formula: C10H9F3O4
SMILES: COc1cccc(OC)c1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 250.17

Physical Properties

Property code	Value	Unit	Source
gf	-899.04	kJ/mol	Joback Method
hf	-1142.46	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.171		Crippen Method
mcvol	152.490	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1287.00		NIST Webbook
tb	580.55	K	Joback Method
tc	774.03	K	Joback Method
tf	374.73	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.42	J/mol×K	580.55	Joback Method
cpg	386.91	J/mol×K	612.80	Joback Method
cpg	397.79	J/mol×K	645.04	Joback Method
cpg	408.08	J/mol×K	677.29	Joback Method
cpg	417.76	J/mol×K	709.54	Joback Method
cpg	426.84	J/mol×K	741.78	Joback Method
cpg	435.32	J/mol×K	774.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374278&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