2,5-Dimethylphenol trifluoroacetate

Inchi: InChI=1S/C10H9F3O2/c1-6-3-4-7(2)8(5-6)15-9(14)10(11,12)13/h3-5H,1-2H3
InchiKey: IBFAGZLTLIKNMS-UHFFFAOYSA-N
Formula: C10H9F3O2
SMILES: Cc1ccc(C)c(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 218.17

Physical Properties

Property code	Value	Unit	Source
gf	-689.04	kJ/mol	Joback Method
hf	-878.02	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	46.86	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.771		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1036.00		NIST Webbook
tb	535.71	K	Joback Method
tc	732.30	K	Joback Method
tf	330.27	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.31	J/mol×K	535.71	Joback Method
cpg	340.22	J/mol×K	568.48	Joback Method
cpg	351.43	J/mol×K	601.24	Joback Method
cpg	361.97	J/mol×K	634.01	Joback Method
cpg	371.86	J/mol×K	666.77	Joback Method
cpg	381.13	J/mol×K	699.54	Joback Method
cpg	389.79	J/mol×K	732.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373030&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