p-Hydroxyphenyllactic acid, TFA-ME

Inchi: InChI=1S/C14H10F6O6/c1-24-10(21)9(26-12(23)14(18,19)20)6-7-2-4-8(5-3-7)25-11(22)1
InchiKey: IUGBOWODUMJWOJ-UHFFFAOYSA-N
Formula: C14H10F6O6
SMILES: COC(=O)C(Cc1ccc(OC(=O)C(F)(F)F)cc1)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 388.22

Physical Properties

Property code	Value	Unit	Source
gf	-1697.60	kJ/mol	Joback Method
hf	-2041.07	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.344		Crippen Method
mcvol	217.300	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
tb	768.97	K	Joback Method
tc	960.49	K	Joback Method
tf	496.34	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.39	J/mol×K	768.97	Joback Method
cpg	642.65	J/mol×K	800.89	Joback Method
cpg	652.06	J/mol×K	832.81	Joback Method
cpg	660.64	J/mol×K	864.73	Joback Method
cpg	668.42	J/mol×K	896.65	Joback Method
cpg	675.44	J/mol×K	928.57	Joback Method
cpg	681.71	J/mol×K	960.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387289&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