p-Hydroxymandelic acid, TFA-ME

Inchi: InChI=1S/C13H8F6O6/c1-23-9(20)8(25-11(22)13(17,18)19)6-2-4-7(5-3-6)24-10(21)12(14
InchiKey: UAMATDKDQXDBOA-UHFFFAOYSA-N
Formula: C13H8F6O6
SMILES: COC(=O)C(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 374.19

Physical Properties

Property code	Value	Unit	Source
gf	-1706.02	kJ/mol	Joback Method
hf	-2020.43	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	67.06	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.474		Crippen Method
mcvol	203.210	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1350.00		NIST Webbook
tb	746.09	K	Joback Method
tc	937.97	K	Joback Method
tf	485.07	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.87	J/mol×K	746.09	Joback Method
cpg	589.72	J/mol×K	778.07	Joback Method
cpg	598.76	J/mol×K	810.05	Joback Method
cpg	607.00	J/mol×K	842.03	Joback Method
cpg	614.47	J/mol×K	874.01	Joback Method
cpg	621.20	J/mol×K	905.99	Joback Method
cpg	627.20	J/mol×K	937.97	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=R387269&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