p-Hydroxyphenylpropionic acid, TFA-ME

Inchi: InChI=1S/C12H11F3O4/c1-18-10(16)7-4-8-2-5-9(6-3-8)19-11(17)12(13,14)15/h2-3,5-6H,
InchiKey: LYFORWVQNRLTOQ-UHFFFAOYSA-N
Formula: C12H11F3O4
SMILES: COC(=O)CCc1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 276.21

Physical Properties

Property code	Value	Unit	Source
gf	-896.49	kJ/mol	Joback Method
hf	-1152.63	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.260		Crippen Method
mcvol	176.370	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	652.78	K	Joback Method
tc	849.33	K	Joback Method
tf	412.45	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.91	J/mol×K	652.78	Joback Method
cpg	475.93	J/mol×K	685.54	Joback Method
cpg	487.17	J/mol×K	718.30	Joback Method
cpg	497.66	J/mol×K	751.06	Joback Method
cpg	507.40	J/mol×K	783.81	Joback Method
cpg	516.43	J/mol×K	816.57	Joback Method
cpg	524.75	J/mol×K	849.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387294&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