3-(4-Hydroxyphenyl)propionic acid, pentafluoropropionate

Inchi: InChI=1S/C12H9F5O4/c13-11(14,12(15,16)17)10(20)21-8-4-1-7(2-5-8)3-6-9(18)19/h1-2,
InchiKey: LAGIHEJEYXGHGM-UHFFFAOYSA-N
Formula: C12H9F5O4
SMILES: O=C(O)CCc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 312.19

Physical Properties

Property code	Value	Unit	Source
gf	-1315.09	kJ/mol	Joback Method
hf	-1573.61	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.807		Crippen Method
mcvol	179.910	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	717.85	K	Joback Method
tc	902.90	K	Joback Method
tf	454.64	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.87	J/mol×K	717.85	Joback Method
cpg	517.08	J/mol×K	748.69	Joback Method
cpg	525.60	J/mol×K	779.53	Joback Method
cpg	533.48	J/mol×K	810.37	Joback Method
cpg	540.76	J/mol×K	841.22	Joback Method
cpg	547.48	J/mol×K	872.06	Joback Method
cpg	553.69	J/mol×K	902.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374903&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