(S)-p-Hydroxyphenyllactic acid, (S)-(+)-3-methyl-2-butyl ester, O-TFA

Inchi: InChI=1S/C18H18F6O6/c1-9(2)10(3)28-14(25)13(30-16(27)18(22,23)24)8-11-4-6-12(7-5

InchiKey: AGEHXNBDEXTKSW-ZWNOBZJWSA-N

Formula: C18H18F6O6

SMILES: CC(C)C(C)OC(=O)C(Cc1ccc(OC(=O)C(F)(F)F)cc1)OC(=O)C(F)(F)F

Mol. weight [g/mol]: 444.32

Physical Properties

Property code	Value	Unit	Source
gf	-1668.80	kJ/mol	Joback Method
hf	-2134.19	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.759		Crippen Method
mcvol	273.660	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	859.61	K	Joback Method
tc	1058.10	K	Joback Method
tf	511.42	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.23	J/mol×K	859.61	Joback Method
cpg	864.94	J/mol×K	892.69	Joback Method
cpg	875.60	J/mol×K	925.77	Joback Method
cpg	885.26	J/mol×K	958.85	Joback Method
cpg	893.95	J/mol×K	991.94	Joback Method
cpg	901.72	J/mol×K	1025.02	Joback Method
cpg	908.60	J/mol×K	1058.10	Joback Method

Sources

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=R601040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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