p-Hydroxyphenylacetic acid, propionyl, DTFMBz

Inchi: InChI=1S/C20H16F6O4/c1-2-17(27)30-16-5-3-12(4-6-16)9-18(28)29-11-13-7-14(19(21,2

InchiKey: SHONDTYPJLMODP-UHFFFAOYSA-N

Formula: C20H16F6O4

SMILES: CCC(=O)Oc1ccc(CC(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1

Mol. weight [g/mol]: 434.33

Physical Properties

Property code	Value	Unit	Source
gf	-1317.57	kJ/mol	Joback Method
hf	-1701.24	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.325		Crippen Method
mcvol	270.640	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2060.00		NIST Webbook
tb	867.04	K	Joback Method
tc	1072.91	K	Joback Method
tf	558.26	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.38	J/mol×K	867.04	Joback Method
cpg	837.08	J/mol×K	901.35	Joback Method
cpg	847.79	J/mol×K	935.66	Joback Method
cpg	857.55	J/mol×K	969.97	Joback Method
cpg	866.44	J/mol×K	1004.29	Joback Method
cpg	874.51	J/mol×K	1038.60	Joback Method
cpg	881.83	J/mol×K	1072.91	Joback Method

Sources

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=R539029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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