p-Hydroxyphenylmandelic acid, acetyl, DTFMBz

Inchi: InChI=1S/C21H16F6O6/c1-11(28)32-17-5-3-14(4-6-17)18(33-12(2)29)19(30)31-10-13-7-

InchiKey: PDAVPCWROSEPFW-UHFFFAOYSA-N

Formula: C21H16F6O6

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

Mol. weight [g/mol]: 478.34

Physical Properties

Property code	Value	Unit	Source
gf	-1545.51	kJ/mol	Joback Method
hf	-1971.96	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.997		Crippen Method
mcvol	292.170	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	965.77	K	Joback Method
tc	1185.40	K	Joback Method
tf	626.69	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.07	J/mol×K	965.77	Joback Method
cpg	925.60	J/mol×K	1002.38	Joback Method
cpg	933.98	J/mol×K	1038.98	Joback Method
cpg	941.25	J/mol×K	1075.59	Joback Method
cpg	947.48	J/mol×K	1112.19	Joback Method
cpg	952.72	J/mol×K	1148.80	Joback Method
cpg	957.04	J/mol×K	1185.40	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=R539034&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