p-Hydroxyphenylacetic acid, acetyl, DTFMBz

Inchi: InChI=1S/C19H14F6O4/c1-11(26)29-16-4-2-12(3-5-16)8-17(27)28-10-13-6-14(18(20,21)
InchiKey: MPHHUIBCLHIUDZ-UHFFFAOYSA-N
Formula: C19H14F6O4
SMILES: CC(=O)Oc1ccc(CC(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1
Mol. weight [g/mol]: 420.30

Physical Properties

Property code	Value	Unit	Source
gf	-1325.99	kJ/mol	Joback Method
hf	-1680.60	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.935		Crippen Method
mcvol	256.550	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	844.16	K	Joback Method
tc	1049.64	K	Joback Method
tf	546.99	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.31	J/mol×K	844.16	Joback Method
cpg	780.74	J/mol×K	878.41	Joback Method
cpg	791.19	J/mol×K	912.65	Joback Method
cpg	800.71	J/mol×K	946.90	Joback Method
cpg	809.37	J/mol×K	981.14	Joback Method
cpg	817.21	J/mol×K	1015.39	Joback Method
cpg	824.31	J/mol×K	1049.64	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=R539014&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