3,4-Dihydroxyphenylacetic acid, acetyl, DTFMBz

Inchi: InChI=1S/C21H16F6O6/c1-11(28)32-17-4-3-13(7-18(17)33-12(2)29)8-19(30)31-10-14-5-

InchiKey: AEYIANKXAZIKOI-UHFFFAOYSA-N

Formula: C21H16F6O6

SMILES: CC(=O)Oc1ccc(CC(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1OC(C)=O

Mol. weight [g/mol]: 478.34

Physical Properties

Property code	Value	Unit	Source
gf	-1552.70	kJ/mol	Joback Method
hf	-1978.15	kJ/mol	Joback Method
hfus	48.68	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.861		Crippen Method
mcvol	292.170	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
tb	971.19	K	Joback Method
tc	1191.02	K	Joback Method
tf	654.21	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.92	J/mol×K	971.19	Joback Method
cpg	923.36	J/mol×K	1007.83	Joback Method
cpg	931.63	J/mol×K	1044.47	Joback Method
cpg	938.79	J/mol×K	1081.10	Joback Method
cpg	944.90	J/mol×K	1117.74	Joback Method
cpg	949.99	J/mol×K	1154.38	Joback Method
cpg	954.12	J/mol×K	1191.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R538942&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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