3,4-Dihydroxyphenylacetic acid, propionyl, DTFMBz

Inchi: InChI=1S/C23H20F6O6/c1-3-19(30)34-17-6-5-13(9-18(17)35-20(31)4-2)10-21(32)33-12-

InchiKey: RBSZVXQBUCQJFA-UHFFFAOYSA-N

Formula: C23H20F6O6

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

Mol. weight [g/mol]: 506.39

Physical Properties

Property code	Value	Unit	Source
gf	-1535.86	kJ/mol	Joback Method
hf	-2019.43	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	93.97	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.641		Crippen Method
mcvol	320.350	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	1016.95	K	Joback Method
tc	1245.03	K	Joback Method
tf	676.75	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.44	J/mol×K	1016.95	Joback Method
cpg	1039.28	J/mol×K	1054.96	Joback Method
cpg	1047.84	J/mol×K	1092.98	Joback Method
cpg	1055.18	J/mol×K	1130.99	Joback Method
cpg	1061.38	J/mol×K	1169.01	Joback Method
cpg	1066.50	J/mol×K	1207.02	Joback Method
cpg	1070.61	J/mol×K	1245.03	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=R538957&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