Dihydroxymandelic acid, acetyl, DTFMBz

Inchi: InChI=1S/C23H18F6O8/c1-11(30)35-18-5-4-15(8-19(18)36-12(2)31)20(37-13(3)32)21(33
InchiKey: FHUZXUCOPLVXSG-UHFFFAOYSA-N
Formula: C23H18F6O8
SMILES: CC(=O)Oc1ccc(C(OC(C)=O)C(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1OC(C)=O
Mol. weight [g/mol]: 536.37

Physical Properties

Property code	Value	Unit	Source
gf	-1772.22	kJ/mol	Joback Method
hf	-2269.51	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	102.73	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	4.922		Crippen Method
mcvol	327.790	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	1092.80	K	Joback Method
tc	1339.30	K	Joback Method
tf	733.91	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.88	J/mol×K	1092.80	Joback Method
cpg	1059.02	J/mol×K	1133.88	Joback Method
cpg	1063.50	J/mol×K	1174.97	Joback Method
cpg	1066.40	J/mol×K	1216.05	Joback Method
cpg	1067.77	J/mol×K	1257.13	Joback Method
cpg	1067.66	J/mol×K	1298.22	Joback Method
cpg	1066.13	J/mol×K	1339.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R538962&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