Dihydroxymandelic acid, propionyl, DTFMBz

Inchi: InChI=1S/C26H24F6O8/c1-4-20(33)38-18-8-7-15(11-19(18)39-21(34)5-2)23(40-22(35)6-
InchiKey: AAGGYOSZFLUBLF-UHFFFAOYSA-N
Formula: C26H24F6O8
SMILES: CCC(=O)Oc1ccc(C(OC(=O)CC)C(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1OC(=O)CC
Mol. weight [g/mol]: 578.45

Physical Properties

Property code	Value	Unit	Source
gf	-1746.96	kJ/mol	Joback Method
hf	-2331.43	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	109.41	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	6.093		Crippen Method
mcvol	370.060	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2519.00		NIST Webbook
tb	1161.44	K	Joback Method
tc	1434.92	K	Joback Method
tf	767.72	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.27	J/mol×K	1161.44	Joback Method
cpg	1232.19	J/mol×K	1207.02	Joback Method
cpg	1236.06	J/mol×K	1252.60	Joback Method
cpg	1237.98	J/mol×K	1298.18	Joback Method
cpg	1238.06	J/mol×K	1343.76	Joback Method
cpg	1236.39	J/mol×K	1389.34	Joback Method
cpg	1233.06	J/mol×K	1434.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R538977&Units=SI

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