Me-dihydrophaseic acid-Ac

Inchi: InChI=1S/C17H24O6/c1-11(7-14(19)20)5-6-17(21)15(3)8-13(23-12(2)18)9-16(17,4)22-10
InchiKey: QYOPWKHLKFNPNL-SVGQIRFLSA-N
Formula: C17H24O6
SMILES: CC(=O)OC1CC2(C)COC(C)(C1)C2(O)C=CC(C)=CC(=O)O
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-413.04	kJ/mol	Joback Method
hf	-825.08	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	103.30	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.825		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	951.43	K	Joback Method
tc	1171.87	K	Joback Method
tf	619.59	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.04	J/mol×K	951.43	Joback Method
cpg	878.41	J/mol×K	988.17	Joback Method
cpg	904.84	J/mol×K	1024.91	Joback Method
cpg	933.67	J/mol×K	1061.65	Joback Method
cpg	965.27	J/mol×K	1098.39	Joback Method
cpg	1000.00	J/mol×K	1135.13	Joback Method
cpg	1038.21	J/mol×K	1171.87	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=R487433&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