5,7-Dihydroxy-2-(p-methoxyphenyl)-6,8-dimethyl-4-(.+/-.)-

Inchi: InChI=1S/C18H18O5/c1-9-16(20)10(2)18-15(17(9)21)13(19)8-14(23-18)11-4-6-12(22-3)7

InchiKey: DZTRDRPCROOSOG-UHFFFAOYSA-N

Formula: C18H18O5

SMILES: COc1ccc(C2CC(=O)c3c(O)c(C)c(O)c(C)c3O2)cc1

Mol. weight [g/mol]: 314.33

CAS: 95273-01-1

Physical Properties

Property code	Value	Unit	Source
gf	-287.32	kJ/mol	Joback Method
hf	-677.57	kJ/mol	Joback Method
hfus	45.18	kJ/mol	Joback Method
hvap	100.14	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.430		Crippen Method
mcvol	231.150	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	2881.20		NIST Webbook
tb	973.96	K	Joback Method
tc	1234.97	K	Joback Method
tf	750.42	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.31	J/mol×K	973.96	Joback Method
cpg	768.16	J/mol×K	1017.46	Joback Method
cpg	782.59	J/mol×K	1060.96	Joback Method
cpg	796.76	J/mol×K	1104.47	Joback Method
cpg	810.82	J/mol×K	1147.97	Joback Method
cpg	824.92	J/mol×K	1191.47	Joback Method
cpg	839.23	J/mol×K	1234.97	Joback Method

Sources

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=C95273011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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