GIBBERELLIC ACID

Other names: (+)-Gibberillic acid

(1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-2,4a,7-Trihydroxy-1-methyl-8-methylg
acid 1,4a-lactone
(3S,3aS,4S,4aS,6S,8aR,8bR,11S)-6,11-dihydroxy-3-methyl-12-methylene-2-oxo-4a,6-eth
2,4a,7-Trihydroxy-1-methyl-8-methylenegibb-3-ene-1,10-dicarboxylic acid,
acid,
1,4a-lactone, (1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-
4a,1-(Epoxymethano)-7,9a-methanobenz[a]azulene, gibb-3-ene-1,10-dicarboxylic
acid deriv.
Activol
Berelex
Brellin
Cekugib
GA
GA3
Gib-Sol
Gib-Tabs
Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-,
1,4a-lactone, (1«alpha»,2«beta»,4a«alpha»,4b«beta»,10«beta»)-
Gibb-tabs
Gibberellic acid GA3
Gibberellin
Gibberellin A3
Gibberellin X
Gibberillic acid
Gibrescol
Gibreskol
Grocel
NCI-C55823
NSC 14190
Pro-Gibb
Pro-Gibb Plus
Regulex
Ryzup

Inchi: InChI=1S/C19H22O6/c1-9-7-17-8-18(9,24)5-3-10(17)19-6-4-11(20)16(2,15(23)25-19)13(

InchiKey: IXORZMNAPKEEDV-UHFFFAOYSA-N

Formula: C19H22O6

SMILES: C=C1CC23CC1(O)CCC2C12C=CC(O)C(C)(C(=O)O1)C2C3C(=O)O

Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source

hfus	30.88	kJ/mol	Joback Method
log10ws	-1.84		Aqueous Solubility Prediction Method
logp	1.027		Crippen Method
mcvol	242.290	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.81	J/mol×K	1086.81	Joback Method
cpg	1086.39	J/mol×K	1127.57	Joback Method
cpg	1141.06	J/mol×K	1168.33	Joback Method
cpg	1202.48	J/mol×K	1209.09	Joback Method
cpg	1271.31	J/mol×K	1249.85	Joback Method
cpg	1348.22	J/mol×K	1290.61	Joback Method
cpg	1433.87	J/mol×K	1331.37	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77065&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume