Gibbane-1,10-dicarboxylic acid, 4a-(hydroxymethyl)-1-methyl-8-methylene-, 1,4a-lactone, 10-methyl ester, (1«alpha»,4a«alpha»,4b«beta»,10«beta»)-

Other names:	4a«alpha»,4b«beta»-Gibbane-1«alpha»,10«beta»-dicarboxylic acid, 4a-(hydroxymethyl)-1-methyl-8-methylene-, 1,4a-lactone, methyl ester Gibberellin A15, methyl ester GA15 ME GA15 methyl ester
Inchi:	InChI=1S/C21H28O4/c1-12-9-21-10-13(12)5-6-14(21)20-8-4-7-19(2,18(23)25-11-20)16(2
InchiKey:	SDNANUVFTHNCBP-UHFFFAOYSA-N
Formula:	C21H28O4
SMILES:	C=C1CC23CC1CCC2C12CCCC(C)(C(=O)OC1)C2C3C(=O)OC
Mol. weight [g/mol]:	344.44
CAS:	13744-19-9

Physical Properties

Property code	Value	Unit	Source
gf	-28.05	kJ/mol	Joback Method
hf	-556.47	kJ/mol	Joback Method
hfus	26.89	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.501		Crippen Method
mcvol	263.030	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2664.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
rinpol	2653.00		NIST Webbook
rinpol	2659.00		NIST Webbook
rinpol	2664.00		NIST Webbook
rinpol	2608.00		NIST Webbook
rinpol	2626.00		NIST Webbook
rinpol	2605.00		NIST Webbook
rinpol	2622.00		NIST Webbook
rinpol	2624.00		NIST Webbook
rinpol	2628.00		NIST Webbook
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook

rinpol	2593.00		NIST Webbook
rinpol	2595.00		NIST Webbook
rinpol	2626.00		NIST Webbook
rinpol	2602.00		NIST Webbook
rinpol	2653.00		NIST Webbook
rinpol	2652.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	887.99	K	Joback Method
tc	1139.83	K	Joback Method
tf	649.42	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.19	J/mol×K	887.99	Joback Method
cpg	983.54	J/mol×K	929.96	Joback Method
cpg	1014.48	J/mol×K	971.94	Joback Method
cpg	1047.57	J/mol×K	1013.91	Joback Method
cpg	1083.38	J/mol×K	1055.88	Joback Method
cpg	1122.47	J/mol×K	1097.86	Joback Method
cpg	1165.40	J/mol×K	1139.83	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=C13744199&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

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