

4a«alpha»,4b«beta»-Gibbane-1«alpha»,10«beta»-acid,

Other names:

2«beta»-OH GA12 methyl ester

Inchi:

InChI=1S/C22H32O5/c1-12-10-22-11-13(12)6-7-14(22)20(2)9-8-15(23)21(3,19(25)27-5)1

SMILES:

CC(=O)OC1C3C(=O)OC(C)(C)C(C)C(C)C1C2C3CC1CCC2C1(C)CCC(O)C(C)(C(=O)OC)C1C3C(=O)OC

Formula:

C22H32O5

SMILES:

C=C1CC23CC1CCC2C1(C)CCC(O)C(C)(C(=O)OC)C1C3C(=O)OC

Mol. weight [g/mol]:

376.49

CAS:

4968-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-257.83	kJ/mol	Joback Method
hf	-817.92	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	95.20	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.108		Crippen Method
mcvol	293.850	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	968.49	K	Joback Method
tc	1195.84	K	Joback Method
tf	672.46	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.06	J/molxK	968.49	Joback Method
cpg	1134.24	J/molxK	1006.38	Joback Method
cpg	1166.22	J/molxK	1044.27	Joback Method
cpg	1200.41	J/molxK	1082.16	Joback Method
cpg	1237.18	J/molxK	1120.06	Joback Method
cpg	1276.93	J/molxK	1157.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4968370&Units=SI
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

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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