4a«alpha»,4b«beta»-Gibbane-1«alpha»,10«beta»-dicarboxylic acid, 1,4a-dimethyl-8-methylene-, dimethyl ester

Other names: Dimethyl 1,4a-dimethyl-8-methylenegibbane-1,10-dicarboxylate, (1«alpha»,4a«alpha»,4b«beta»,10«beta»)-, GA12, Me

GA12 methyl ester

Inchi: InChI=1S/C22H32O4/c1-13-11-22-12-14(13)7-8-15(22)20(2)9-6-10-21(3,19(24)26-5)17(2

InchiKey: PWWAKLGQWQLLIY-UHFFFAOYSA-N

Formula: C22H32O4

SMILES: C=C1CC23CC1CCC2C1(C)CCCC(C)(C(=O)OC)C1C3C(=O)OC

Mol. weight [g/mol]: 360.49

CAS: 22882-62-8

Physical Properties

Property code	Value	Unit	Source
gf	-113.30	kJ/mol	Joback Method
hf	-645.35	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	78.83	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.137		Crippen Method
mcvol	287.980	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2329.00		NIST Webbook
rinpol	2328.00		NIST Webbook
rinpol	2329.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2346.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2323.00		NIST Webbook
rinpol	2332.00		NIST Webbook

rinpol	2326.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2371.00		NIST Webbook
rinpol	2344.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2369.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2326.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	880.98	K	Joback Method
tc	1113.24	K	Joback Method
tf	615.88	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.49	J/mol×K	880.98	Joback Method
cpg	1042.28	J/mol×K	919.69	Joback Method
cpg	1071.10	J/mol×K	958.40	Joback Method
cpg	1101.38	J/mol×K	997.11	Joback Method
cpg	1133.54	J/mol×K	1035.82	Joback Method
cpg	1168.00	J/mol×K	1074.53	Joback Method
cpg	1205.18	J/mol×K	1113.24	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=C22882628&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