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

Other names: Dimethyl 4a-formyl-1-methyl-8-methylenegibbane-1,10-dicarboxylate, (1«alpha»,4a«alpha»,4b«beta»,10«beta»)-, GA24, Me

InChI: InChI=1S/C22H30O5/c1-13-10-22-11-14(13)6-7-15(22)21(12-23)9-5-8-20(2,19(25)27-4)16(21)17(22)18(24)26-3

InchiKey: CDZKHHKZGGMPOC-UHFFFAOYSA-N

Formula: C22H30O5

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

Mol. weight [g/mol]: 374.47

CAS: 19427-33-9

Physical Properties

Property code	Value	Unit	Source
gf	-212.82	kJ/mol	Joback Method
hf	-730.93	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.317		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2440.00		NIST Webbook
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
rinpol	2477.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
rinpol	2451.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	929.64	K	Joback Method

tc	1164.39	K	Joback Method
tf	657.88	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.61	J/mol×K	929.64	Joback Method
cpg	1070.38	J/mol×K	968.77	Joback Method
cpg	1100.77	J/mol×K	1007.89	Joback Method
cpg	1133.19	J/mol×K	1047.02	Joback Method
cpg	1168.10	J/mol×K	1086.14	Joback Method
cpg	1205.91	J/mol×K	1125.27	Joback Method
cpg	1247.07	J/mol×K	1164.39	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=C19427339&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