

9,15-cyclo-GA9 (GA103), Me

Other names:	GA103, Methyl ester
Inchi:	InChI=1S/C20H24O4/c1-10-11-5-8-19-13(10)18(19,9-11)12(15(21)23-3)14-17(2)6-4-7-20
InchiKey:	GABCKUAZOCTIQC-XQZKAHCQSA-N
Formula:	C20H24O4
SMILES:	<chem>C=C1C2CCC34C1C3(C2)C(C(=O)OC)C1C2(C)CCCC14OC2=O</chem>
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	67.19	kJ/mol	Joback Method
hf	-423.15	kJ/mol	Joback Method
hfus	24.53	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.864		Crippen Method
mcvol	238.080	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2251.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2251.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	855.01	K	Joback Method
tc	1106.57	K	Joback Method
tf	694.07	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.65	J/molxK	855.01	Joback Method
cpg	881.12	J/molxK	896.94	Joback Method
cpg	912.41	J/molxK	938.86	Joback Method
cpg	947.29	J/molxK	980.79	Joback Method

cpg	986.56	J/mol×K	1022.72	Joback Method
cpg	1030.99	J/mol×K	1064.65	Joback Method
cpg	1081.38	J/mol×K	1106.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224292&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mvol:	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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