

Cis Megastigma-5,8-diene-4-one

Inchi:	InChI=1S/C13H20O/c1-5-6-7-11-10(2)12(14)8-9-13(11,3)4/h5-6H,7-9H2,1-4H3/b6-5-
InchiKey:	CVDHBGKYPTUEAA-WAYWQWQTSA-N
Formula:	C13H20O
SMILES:	CC=CCC1=C(C)C(=O)CCC1(C)C
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	45.87	kJ/mol	Joback Method
hf	-227.73	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	49.63	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
tb	597.73	K	Joback Method
tc	822.54	K	Joback Method
tf	356.49	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.71	J/mol×K	597.73	Joback Method
cpg	466.32	J/mol×K	635.20	Joback Method
cpg	483.96	J/mol×K	672.67	Joback Method
cpg	500.76	J/mol×K	710.14	Joback Method
cpg	516.80	J/mol×K	747.60	Joback Method
cpg	532.21	J/mol×K	785.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R440192&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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