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/h5H,1,6-9H2,2-4H3
InchiKey: CZQIKCBGQZBANA-UHFFFAOYSA-N
Formula: C13H20O
SMILES: C=CCCC1=C(C)C(=O)CCC1(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	53.49	kJ/mol	Joback Method
hf	-219.52	kJ/mol	Joback Method
hfus	13.64	kJ/mol	Joback Method
hvap	49.00	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
tb	590.25	K	Joback Method
tc	810.12	K	Joback Method
tf	359.81	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.49	J/mol×K	590.25	Joback Method
cpg	464.93	J/mol×K	626.89	Joback Method
cpg	482.43	J/mol×K	663.54	Joback Method
cpg	499.10	J/mol×K	700.18	Joback Method
cpg	515.02	J/mol×K	736.83	Joback Method
cpg	530.29	J/mol×K	773.47	Joback Method

cpg	544.99	J/mol×K	810.12	Joback Method

Sources

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=R637128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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