

Megastigmatrienone

Inchi:	InChI=1S/C13H18O/c1-5-6-7-12-10(2)8-11(14)9-13(12,3)4/h5-8,12H,1,9H2,2-4H3/b7-6+
InchiKey:	YKVWPZJHENXDAJ-VOTSOKGWSA-N
Formula:	C13H18O
SMILES:	<chem>C=CC=CC1C(C)=CC(=O)CC1(C)C</chem>
Mol. weight [g/mol]:	190.28
CAS:	38818-55-2

Physical Properties

Property code	Value	Unit	Source
gf	135.63	kJ/mol	Joback Method
hf	-111.17	kJ/mol	Joback Method
hfus	15.30	kJ/mol	Joback Method
hvap	47.99	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.290		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	584.76	K	Joback Method
tc	813.41	K	Joback Method
tf	337.97	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.27	J/molxK	584.76	Joback Method
cpg	447.05	J/molxK	622.87	Joback Method
cpg	464.77	J/molxK	660.98	Joback Method
cpg	481.55	J/molxK	699.08	Joback Method
cpg	497.51	J/molxK	737.19	Joback Method

cpg	512.77	J/mol×K	775.30	Joback Method
cpg	527.45	J/mol×K	813.41	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=C38818552&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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