Megastigma-4,6(E),8(Z)-triene

Other names:	Cyclohexene, 6-(2-butenylidene)-1,5,5-trimethyl-, (E,Z)- megastigme-4,6(E),8(Z)-triene 6-[2-Butenylidene]-1,5,5-trimethyl-1-cyclohexene, (E,Z)-isomer Cyclohexene, 6-(2Z)-2-buten-1-ylidene-1,5,5-trimethyl-, (6E)-
Inchi:	InChI=1S/C13H20/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-6,8-9H,7,10H2,1-4H3/b6-5+,12-
InchiKey:	BYDQKMZEOZVIJM-HFACTSAFSA-N
Formula:	C13H20
SMILES:	CC=CC=C1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	176.30
CAS:	71186-24-8

Physical Properties

Property code	Value	Unit	Source
gf	223.55	kJ/mol	Joback Method
hf	-2.53	kJ/mol	Joback Method
hfus	16.32	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1343.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook
tb	531.57	K	Joback Method
tc	748.41	K	Joback Method
tf	286.11	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	394.30	J/mol×K	531.57	Joback Method
cpg	413.03	J/mol×K	567.71	Joback Method
cpg	430.58	J/mol×K	603.85	Joback Method
cpg	447.07	J/mol×K	639.99	Joback Method
cpg	462.65	J/mol×K	676.13	Joback Method
cpg	477.45	J/mol×K	712.27	Joback Method
cpg	491.60	J/mol×K	748.41	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=C71186248&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

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