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

Other names: Cyclohexene, 6-(2-butenylidene)-1,5,5-trimethyl-, (E,E)-
1-(But-2-enylidene)-2,6,6-trimethylcyclohex-2-ene, (E,E)-
Megastigme-4,6(E),8(E)-triene
6-[2-Butenylidene]-1,5,5-trimethyl-1-cyclohexene, (E,E)-
Cyclohexene, 6-(2E)-2-buten-1-ylidene-1,5,5-trimethyl-, (6E)-
1-(but-2-enylidene)-2,6,6-trimethylcyclohex-2-ene[megastigma-4,6(E),8(E)-triene]

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: 51468-86-1

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	1315.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1360.00		NIST Webbook
ripol	1568.00		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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C51468861&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