

(2S,6R,7S,8E)-(+)-2,7-Epoxy-4,8-megastigmadiene

Other names:	2,7-Epoxy-megastigma-4,8-diene
Inchi:	InChI=1S/C13H20O/c1-5-6-10-12-9(2)7-8-11(14-10)13(12,3)4/h5-7,10-12H,8H2,1-4H3/b
InchiKey:	DUQZZCOYQGZPEG-AATRIKPKSA-N
Formula:	C13H20O
SMILES:	CC=CC1OC2CC=C(C)C1C2(C)C
Mol. weight [g/mol]:	192.30
CAS:	108342-25-2

Physical Properties

Property code	Value	Unit	Source
gf	149.40	kJ/mol	Joback Method
hf	-172.28	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.322		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
ripol	2187.00		NIST Webbook
ripol	2187.00		NIST Webbook
tb	545.01	K	Joback Method
tc	760.98	K	Joback Method
tf	315.30	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.31	J/molxK	545.01	Joback Method
cpg	452.20	J/molxK	581.01	Joback Method
cpg	470.80	J/molxK	617.00	Joback Method
cpg	488.26	J/molxK	653.00	Joback Method
cpg	504.73	J/molxK	688.99	Joback Method
cpg	520.37	J/molxK	724.99	Joback Method

Sources

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=C108342252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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