MEGASTIGMA-4,6(Z),8(Z)-TRIENE

Other names: megastigme-4,6(Z),8(Z)-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-FPONQXLSSA-N
Formula: C13H20
SMILES: C/C=C/C=C1/C(C)=CCCC1(C)C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
hf	43.38	kJ/mol	Cheméo Relay (1.0)
hfus	16.32	kJ/mol	Joback Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
rinpol	1324.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
ripol	1606.00		NIST Webbook

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71186259&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices