(2S,6R,7S,8E)-(+)-2,7-EPOXY-4,8-MEGASTIGMADI

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: C/C=C/C1OC2CC=C(C)C1C2(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	26.35	kJ/mol	Joback Method
logp	3.322		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
ripol	2187.00		NIST Webbook
ripol	2187.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.31	J/mol×K	545.01	Joback Method
cpg	452.20	J/mol×K	581.01	Joback Method
cpg	470.80	J/mol×K	617.00	Joback Method
cpg	488.26	J/mol×K	653.00	Joback Method
cpg	504.73	J/mol×K	688.99	Joback Method
cpg	520.37	J/mol×K	724.99	Joback Method
cpg	535.32	J/mol×K	760.98	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108342252&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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