6,12-Epoxyelema-1,3-diene

Inchi: InChI=1S/C15H24O/c1-6-15(5)8-7-12-11(4)9-16-14(12)13(15)10(2)3/h6,11-14H,1-2,7-9H
InchiKey: WHGDEUFMJMWQGK-ZQNQSHIBSA-N
Formula: C15H24O
SMILES: C=CC1(C)CCC2C(C)COC2C1C(=C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	213.01	kJ/mol	Joback Method
hf	-162.52	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	50.50	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.816		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1960.00		NIST Webbook
tb	575.31	K	Joback Method
tc	791.69	K	Joback Method
tf	304.40	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.43	J/mol×K	575.31	Joback Method
cpg	556.69	J/mol×K	611.37	Joback Method
cpg	578.53	J/mol×K	647.44	Joback Method
cpg	599.11	J/mol×K	683.50	Joback Method
cpg	618.55	J/mol×K	719.56	Joback Method
cpg	637.02	J/mol×K	755.63	Joback Method

cpg	654.65	J/mol×K	791.69	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=R198782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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