7,11;8,12-Diepoxy-eremophil-9-ene (epimer A)

Inchi: InChI=1S/C15H22O2/c1-10-5-4-6-11-7-12-15(8-13(10,11)2)14(3,17-15)9-16-12/h7,10,12
InchiKey: LHTGLYLMFOPXAB-NFPJTLMNSA-N
Formula: C15H22O2
SMILES: CC1CCCC2=CC3OCC4(C)OC34CC21C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	118.13	kJ/mol	Joback Method
hf	-266.36	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.069		Crippen Method
mcvol	186.210	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	632.19	K	Joback Method
tc	878.01	K	Joback Method
tf	457.41	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.18	J/mol×K	632.19	Joback Method
cpg	576.02	J/mol×K	673.16	Joback Method
cpg	595.77	J/mol×K	714.13	Joback Method
cpg	614.98	J/mol×K	755.10	Joback Method
cpg	634.20	J/mol×K	796.07	Joback Method
cpg	653.98	J/mol×K	837.04	Joback Method
cpg	674.87	J/mol×K	878.01	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=R236116&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume