7,10-Epoxy-eremophila-1,11-diene

Inchi: InChI=1S/C15H22O/c1-11(2)14-8-9-15(16-14)7-5-6-12(3)13(15,4)10-14/h5,7,12H,1,6,8-1
InchiKey: QDVFFOQYCXJEMT-LJISPDSOSA-N
Formula: C15H22O
SMILES: C=C(C)C12CCC3(C=CCC(C)C3(C)C1)O2
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	232.42	kJ/mol	Joback Method
hf	-80.05	kJ/mol	Joback Method
hfus	13.60	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	1497.00		NIST Webbook
tb	590.08	K	Joback Method
tc	830.63	K	Joback Method
tf	384.66	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.13	J/mol×K	590.08	Joback Method
cpg	535.34	J/mol×K	630.17	Joback Method
cpg	555.05	J/mol×K	670.26	Joback Method
cpg	573.73	J/mol×K	710.36	Joback Method
cpg	591.90	J/mol×K	750.45	Joback Method
cpg	610.06	J/mol×K	790.54	Joback Method
cpg	628.69	J/mol×K	830.63	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=R198831&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume