7-«alpha»-H-Eremophila-1(10),4(15)-dien-2-«alpha» methyl ether

Inchi: InChI=1S/C16H26O/c1-11(2)13-6-7-14-9-15(17-5)8-12(3)16(14,4)10-13/h9,11,13,15H,3,6

InchiKey: YBDXWBCELMMYLN-IMJJTQAJSA-N

Formula: C16H26O

SMILES: C=C1CC(OC)C=C2CCC(C(C)C)CC12C

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	109.71	kJ/mol	Joback Method
hf	-264.66	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	53.40	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.350		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1650.00		NIST Webbook
tb	616.89	K	Joback Method
tc	833.05	K	Joback Method
tf	345.73	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.78	J/mol×K	616.89	Joback Method
cpg	606.30	J/mol×K	652.92	Joback Method
cpg	627.59	J/mol×K	688.94	Joback Method
cpg	647.78	J/mol×K	724.97	Joback Method
cpg	666.99	J/mol×K	761.00	Joback Method
cpg	685.33	J/mol×K	797.02	Joback Method
cpg	702.92	J/mol×K	833.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236141&Units=SI
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

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