E-Eremophila-1(10),7(11)-dien-12-yl methyl ether

Inchi: InChI=1S/C16H26O/c1-12(11-17-4)14-8-9-15-7-5-6-13(2)16(15,3)10-14/h7,13H,5-6,8-11

InchiKey: QXOBNGNKLWIWPZ-WMGVVHKYSA-N

Formula: C16H26O

SMILES: COCC(C)=C1CCC2=CCCC(C)C2(C)C1

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	103.69	kJ/mol	Joback Method
hf	-257.04	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	54.80	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.496		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
ripol	2112.00		NIST Webbook
ripol	2112.00		NIST Webbook
tb	629.36	K	Joback Method
tc	849.45	K	Joback Method
tf	347.69	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.03	J/mol×K	629.36	Joback Method
cpg	606.03	J/mol×K	666.04	Joback Method
cpg	626.82	J/mol×K	702.72	Joback Method
cpg	646.55	J/mol×K	739.40	Joback Method
cpg	665.35	J/mol×K	776.08	Joback Method
cpg	683.39	J/mol×K	812.77	Joback Method

cpg	700.78	J/mol×K	849.45	Joback Method

Sources

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=R236176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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