Eremophila-1(10),7(11)-dien-2-«alpha»-yl 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/h9,12,15H,6-8,1

InchiKey: BIPWPPDODKZLJM-WQVCFCJDSA-N

Formula: C16H26O

SMILES: COC1C=C2CCC(=C(C)C)CC2(C)C(C)C1

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	95.98	kJ/mol	Joback Method
hf	-277.38	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.494		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1715.00		NIST Webbook
tb	624.69	K	Joback Method
tc	844.78	K	Joback Method
tf	343.45	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.28	J/mol×K	624.69	Joback Method
cpg	607.80	J/mol×K	661.37	Joback Method
cpg	629.09	J/mol×K	698.05	Joback Method
cpg	649.30	J/mol×K	734.74	Joback Method
cpg	668.54	J/mol×K	771.42	Joback Method
cpg	686.97	J/mol×K	808.10	Joback Method
cpg	704.71	J/mol×K	844.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236181&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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