

Eudesma-3,5-dien-1 «alpha»-yl methyl ether

Inchi:	InChI=1S/C16H26O/c1-11(2)13-8-9-16(4)14(10-13)12(3)6-7-15(16)17-5/h6,10-11,13,15H
InchiKey:	LVFDEVYJMMYOB-NUEKZKHPSA-N
Formula:	C16H26O
SMILES:	<chem>COC1CC=C(C)C2=CC(C(C)C)CCC21C</chem>
Mol. weight [g/mol]:	234.38

Physical Properties

Property code	Value	Unit	Source
gf	76.96	kJ/mol	Joback Method
hf	-302.59	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.350		Crippen Method
mvol	211.850	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
ripol	1645.00		NIST Webbook
ripol	1967.00		NIST Webbook
tb	621.87	K	Joback Method
tc	839.15	K	Joback Method
tf	345.33	K	Joback Method
vc	0.794	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.15	J/mol×K	621.87	Joback Method
cpg	607.46	J/mol×K	658.08	Joback Method
cpg	628.57	J/mol×K	694.30	Joback Method
cpg	648.59	J/mol×K	730.51	Joback Method
cpg	667.65	J/mol×K	766.72	Joback Method
cpg	685.88	J/mol×K	802.94	Joback Method
cpg	703.39	J/mol×K	839.15	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=R236196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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