

Ziza-6(13)en-3«alpha»-yl methyl ether

Inchi:	InChI=1S/C16H26O/c1-10-13-8-14(17-5)11(2)16(13)7-6-12(9-16)15(10,3)4/h11-14H,1,6-
InchiKey:	SSGKVXFRAKOLHP-RGRSPFQKSA-N
Formula:	C16H26O
SMILES:	C=C1C2CC(OC)C(C)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	234.38

Physical Properties

Property code	Value	Unit	Source
gf	155.86	kJ/mol	Joback Method
hf	-246.01	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	4.040		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
ripol	1626.00		NIST Webbook
ripol	1982.00		NIST Webbook
ripol	1982.00		NIST Webbook
tb	602.29	K	Joback Method
tc	819.75	K	Joback Method
tf	387.85	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.98	J/molxK	602.29	Joback Method
cpg	609.12	J/molxK	638.53	Joback Method
cpg	630.98	J/molxK	674.78	Joback Method
cpg	651.78	J/molxK	711.02	Joback Method
cpg	671.78	J/molxK	747.26	Joback Method
cpg	691.20	J/molxK	783.51	Joback Method
cpg	710.30	J/molxK	819.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R236314&Units=SI

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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