

Ziza-5-en-12-yl methyl ether

Inchi:	InChI=1S/C16H26O/c1-11-5-6-14-12(2)15(3,10-17-4)13-7-8-16(11,14)9-13/h11,13H,5-10
InchiKey:	NRQSCFQEHCWQB-ORLVNTPVSA-N
Formula:	C16H26O
SMILES:	COCC1(C)C(C)=C2CCC(C)C23CCC1C3
Mol. weight [g/mol]:	234.38

Physical Properties

Property code	Value	Unit	Source
gf	128.90	kJ/mol	Joback Method
hf	-254.73	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.186		Crippen Method
mvol	205.290	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	621.59	K	Joback Method
tc	841.16	K	Joback Method
tf	408.45	K	Joback Method
vc	0.785	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.68	J/mol×K	621.59	Joback Method
cpg	607.31	J/mol×K	658.19	Joback Method
cpg	627.82	J/mol×K	694.78	Joback Method
cpg	647.46	J/mol×K	731.38	Joback Method
cpg	666.49	J/mol×K	767.97	Joback Method
cpg	685.19	J/mol×K	804.57	Joback Method
cpg	703.80	J/mol×K	841.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R501430&Units=SI

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

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