

Ziza-6(13)-en-12-yl methyl ether

Inchi:	InChI=1S/C16H26O/c1-11-14-6-5-13(10-17-4)16(14)8-7-12(9-16)15(11,2)3/h12-14H,1,5-
InchiKey:	KPAXHRFTWMHQDO-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	C=C1C2CCC(COC)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	234.38
CAS:	300349-20-6

Physical Properties

Property code	Value	Unit	Source
gf	163.57	kJ/mol	Joback Method
hf	-225.67	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.042		Crippen Method
mcvol	205.290	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1661.60		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1661.60		NIST Webbook
rinpol	1650.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1991.00		NIST Webbook
tb	606.96	K	Joback Method
tc	824.44	K	Joback Method
tf	392.09	K	Joback Method
vc	0.782	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	585.07	J/mol×K	606.96	Joback Method
cpg	607.69	J/mol×K	643.21	Joback Method
cpg	629.04	J/mol×K	679.45	Joback Method
cpg	649.38	J/mol×K	715.70	Joback Method
cpg	668.95	J/mol×K	751.95	Joback Method
cpg	688.01	J/mol×K	788.19	Joback Method
cpg	706.80	J/mol×K	824.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C300349206&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

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

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