

Ziza-6(13)-en-3-one

Other names:	Ziza-6(13)-en-3-one (methyl group in 2-«beta»-position)
Inchi:	InChI=1S/C15H22O/c1-9-12-7-13(16)10(2)15(12)6-5-11(8-15)14(9,3)4/h10-12H,1,5-8H2
InchiKey:	RVQOGXCBZWSGSS-OUEWMDHJSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1C2CC(=O)C(C)C23CCC(C3)C1(C)C</chem>
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	137.56	kJ/mol	Joback Method
hf	-210.51	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	50.55	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	629.48	K	Joback Method
tc	866.95	K	Joback Method
tf	426.81	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.93	J/molxK	629.48	Joback Method
cpg	563.88	J/molxK	669.06	Joback Method
cpg	584.68	J/molxK	708.64	Joback Method

cpg	604.63	J/mol×K	748.22	Joback Method
cpg	624.03	J/mol×K	787.79	Joback Method
cpg	643.18	J/mol×K	827.37	Joback Method
cpg	662.38	J/mol×K	866.95	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=R199418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.chemeo.com/cid/12-157-4/Ziza-6-13-en-3-one.pdf>

Generated by Cheméo on 2024-04-26 14:21:35.313423017 +0000 UTC m=+16430544.234000332.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.