

Ziza-5-en-12-ol

Inchi:	InChI=1S/C15H24O/c1-10-13-5-4-12(9-16)15(13)7-6-11(8-15)14(10,2)3/h11-12,16H,4-9H
InchiKey:	VBWJNOSNXFRVTL-SLEUVZQESA-N
Formula:	C15H24O
SMILES:	CC1=C2CCC(CO)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	88.66	kJ/mol	Joback Method
hf	-254.10	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.531		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinsol	1713.00		NIST Webbook
tb	668.47	K	Joback Method
tc	878.17	K	Joback Method
tf	435.77	K	Joback Method
vc	0.731	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.20	J/mol×K	668.47	Joback Method
cpg	590.05	J/mol×K	703.42	Joback Method
cpg	607.23	J/mol×K	738.37	Joback Method
cpg	623.97	J/mol×K	773.32	Joback Method
cpg	640.53	J/mol×K	808.27	Joback Method
cpg	657.13	J/mol×K	843.22	Joback Method
cpg	674.02	J/mol×K	878.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566006&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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