

12-nor-Ziza-6(13)-en-2«alpha»-ol

Inchi:	InChI=1S/C14H22O/c1-9-11-4-5-12(15)14(11)7-6-10(8-14)13(9,2)3/h10-12,15H,1,4-8H2,
InchiKey:	CXANYYGAWHHNM-XVXXKJFYSA-N
Formula:	C14H22O
SMILES:	C=C1C2CCC(O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	114.91	kJ/mol	Joback Method
hf	-204.40	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.140		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	630.96	K	Joback Method
tc	841.94	K	Joback Method
tf	408.14	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.51	J/mol×K	630.96	Joback Method
cpg	538.69	J/mol×K	666.12	Joback Method
cpg	555.95	J/mol×K	701.29	Joback Method
cpg	572.53	J/mol×K	736.45	Joback Method
cpg	588.66	J/mol×K	771.61	Joback Method
cpg	604.59	J/mol×K	806.77	Joback Method
cpg	620.56	J/mol×K	841.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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