

15-nor-Prezizaan-7a-ol

Inchi:	InChI=1S/C14H24O/c1-9-4-5-11-13(2,3)12(15)10-6-7-14(9,11)8-10/h9-12,15H,4-8H2,1-3
InchiKey:	RJTVRURTSNYWOY-YWDZHIDKSA-N
Formula:	C14H24O
SMILES:	CC1CCC2C(C)(C)C(O)C3CCC12C3
Mol. weight [g/mol]:	208.34

Physical Properties

Property code	Value	Unit	Source
gf	54.12	kJ/mol	Joback Method
hf	-308.98	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	60.29	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.220		Crippen Method
mcvol	181.410	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	627.13	K	Joback Method
tc	836.42	K	Joback Method
tf	390.22	K	Joback Method
vc	0.686	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.87	J/mol×K	627.13	Joback Method
cpg	564.57	J/mol×K	662.01	Joback Method
cpg	583.25	J/mol×K	696.89	Joback Method
cpg	601.15	J/mol×K	731.78	Joback Method
cpg	618.50	J/mol×K	766.66	Joback Method
cpg	635.52	J/mol×K	801.54	Joback Method
cpg	652.46	J/mol×K	836.42	Joback Method

Sources

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=R397830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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