

1H-Inden-3-ol, 2,3,3a,4,5,6-hexahydro-2,2-dimethyl-5-methylene-

Inchi:	InChI=1S/C13H20O2/c1-8-4-9(7-14)11-6-13(2,3)12(15)10(11)5-8/h10,12,14-15H,1,4-7H2
InchiKey:	VCIVBLZCBOWLMD-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	C=C1CC(CO)=C2CC(C)(C)C(O)C2C1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	-79.28	kJ/mol	Joback Method
hf	-375.01	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.032		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpole	1849.00		NIST Webbook
ripole	3118.00		NIST Webbook
ripole	3118.00		NIST Webbook
tb	711.34	K	Joback Method
tc	904.56	K	Joback Method
tf	442.37	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.67	J/molxK	711.34	Joback Method
cpg	537.43	J/molxK	743.54	Joback Method
cpg	550.68	J/molxK	775.75	Joback Method
cpg	563.53	J/molxK	807.95	Joback Method
cpg	576.07	J/molxK	840.16	Joback Method
cpg	588.38	J/molxK	872.36	Joback Method
cpg	600.57	J/molxK	904.56	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=R546448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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