

1H-Inden-7-ol, 2,6,7,7a-tetrahydro, 2,2,7-trimethyl-5-hydroxymethyl-6-cyclopropano

Inchi:	InChI=1S/C15H22O2/c1-13(2)7-10-6-11(9-16)15(4-5-15)14(3,17)12(10)8-13/h6-7,12,16-
InchiKey:	YEDYYAKSTVQMBN-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CC1(C)C=C2C=C(CO)C3(CC3)C(C)(O)C2C1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	-23.69	kJ/mol	Joback Method
hf	-333.31	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.422		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1856.00		NIST Webbook
ripol	2985.00		NIST Webbook
tb	760.05	K	Joback Method
tc	966.03	K	Joback Method
tf	521.25	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.97	J/molxK	760.05	Joback Method
cpg	620.59	J/molxK	794.38	Joback Method
cpg	636.62	J/molxK	828.71	Joback Method
cpg	653.36	J/molxK	863.04	Joback Method
cpg	671.12	J/molxK	897.37	Joback Method
cpg	690.20	J/molxK	931.70	Joback Method
cpg	710.90	J/molxK	966.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R546468&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
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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