

1H-Inden-1-ol, 2,3-dihydro-3,3-dimethyl-

Other names:	1-Indanol, 3,3-dimethyl- 3,3-Dimethyl-1-indanol
Inchi:	InChI=1S/C11H14O/c1-11(2)7-10(12)8-5-3-4-6-9(8)11/h3-6,10,12H,7H2,1-2H3
InchiKey:	JYSNWEPTBXFJSP-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC1(C)CC(O)c2ccccc21
Mol. weight [g/mol]:	162.23
CAS:	38393-92-9

Physical Properties

Property code	Value	Unit	Source
gf	55.25	kJ/mol	Joback Method
hf	-129.84	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.401		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	577.23	K	Joback Method
tc	789.31	K	Joback Method
tf	351.09	K	Joback Method
vc	0.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.74	J/molxK	577.23	Joback Method
cpg	357.31	J/molxK	612.58	Joback Method
cpg	370.01	J/molxK	647.92	Joback Method
cpg	381.97	J/molxK	683.27	Joback Method
cpg	393.32	J/molxK	718.62	Joback Method
cpg	404.20	J/molxK	753.96	Joback Method
cpg	414.73	J/molxK	789.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38393929&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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