

1H-Inden-2-ol, 2,3-dihydro-1-methoxy-, cis-

Other names:	1-Methoxy-2-indanol
Inchi:	InChI=1S/C10H12O2/c1-12-10-8-5-3-2-4-7(8)6-9(10)11/h2-5,9-11H,6H2,1H3/t9-,10+/m1
InchiKey:	ZHWPZRVYPHGXSf-ZJUuuORDSA-N
Formula:	C10H12O2
SMILES:	COC1c2ccccc2CC1O
Mol. weight [g/mol]:	164.20
CAS:	56175-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-52.68	kJ/mol	Joback Method
hf	-256.66	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	59.48	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.291		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	576.53	K	Joback Method
tc	781.79	K	Joback Method
tf	338.15	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.47	J/mol×K	576.53	Joback Method
cpg	379.88	J/mol×K	747.58	Joback Method
cpg	369.78	J/mol×K	713.37	Joback Method
cpg	359.02	J/mol×K	679.16	Joback Method
cpg	347.57	J/mol×K	644.95	Joback Method
cpg	335.40	J/mol×K	610.74	Joback Method
cpg	389.36	J/mol×K	781.79	Joback Method
dvisc	0.0001970	Pa×s	576.53	Joback Method

dvisc	0.0002651	Pa×s	536.80	Joback Method
dvisc	0.0003741	Pa×s	497.07	Joback Method
dvisc	0.0005604	Pa×s	457.34	Joback Method
dvisc	0.0009066	Pa×s	417.61	Joback Method
dvisc	0.0016228	Pa×s	377.88	Joback Method
dvisc	0.0033304	Pa×s	338.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	1.50	NIST Webbook

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=C56175441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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