1H-Indene-1,2-diol, 2,3-dihydro-, trans-

Other names:	1,2-Indandiol, trans-
	trans-1,2-Dihydroxyindane
	trans-1,2-Indandiol
	(E)-1,2-Indanediol
Inchi:	InChI=1S/C9H10O2/c10-8-5-6-3-1-2-4-7(6)9(8)11/h1-4,8-11H,5H2/t8-,9-/m0/s1
InchiKey:	YKXXBEOXRPZVCC-IUCAKERBSA-N
Formula:	C9H10O2
SMILES:	OC1Cc2ccccc2C1O
Mol. weight [g/mol]:	150.17
CAS:	4647-43-2

Physical Properties

Property code	Value	Unit	Source
chs	-4585.00 ± 2.00	kJ/mol	NIST Webbook
gf	-92.92	kJ/mol	Joback Method
hf	-256.03	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	71.53	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.637		Crippen Method
mcvol	114.790	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	623.41	K	Joback Method
tc	820.36	K	Joback Method
tf	365.47	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.01	J/mol×K	623.41	Joback Method
cpg	310.98	J/mol×K	656.23	Joback Method
cpg	320.34	J/mol×K	689.06	Joback Method
cpg	329.11	J/mol×K	721.88	Joback Method

cpg	337.35	J/mol×K	754.71	Joback Method
cpg	345.09	J/mol×K	787.53	Joback Method
cpg	352.37	J/mol×K	820.36	Joback Method
dvisc	0.0058361	Pa×s	365.47	Joback Method
dvisc	0.0019449	Pa×s	408.46	Joback Method
dvisc	0.0007990	Pa×s	451.45	Joback Method
dvisc	0.0003832	Pa×s	494.44	Joback Method
dvisc	0.0002067	Pa×s	537.43	Joback Method
dvisc	0.0001222	Pa×s	580.42	Joback Method
dvisc	0.0000776	Pa×s	623.41	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4647432&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

chs: Standard solid enthalpy of combustion
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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