1,2,3,6,7,8-Hexahydro-as-indacene

Other names: As-Indacene,1,2,3,6,7,8-hexahydro-
1,2,3,6,7,8-Hexahydro-cis-indacene
Inchi: InChI=1S/C12H14/c1-3-9-7-8-10-4-2-6-12(10)11(9)5-1/h7-8H,1-6H2
InchiKey: CGIPSWGAIQVCNY-UHFFFAOYSA-N
Formula: C12H14
SMILES: c1cc2c(c3c1CCC3)CCC2
Mol. weight [g/mol]: 158.24
CAS: 1076-17-1

Physical Properties

Property code	Value	Unit	Source
gf	270.60	kJ/mol	Joback Method
hf	97.39	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
ie	8.09	eV	NIST Webbook
ie	8.66 ± 0.02	eV	NIST Webbook
log10ws	-3.63		Crippen Method
logp	2.664		Crippen Method
mcvol	134.460	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	538.40	K	Joback Method
tc	774.59	K	Joback Method
tf	333.34	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.68	J/mol×K	538.40	Joback Method
cpg	389.15	J/mol×K	735.23	Joback Method
cpg	376.80	J/mol×K	695.86	Joback Method
cpg	363.50	J/mol×K	656.50	Joback Method
cpg	349.13	J/mol×K	617.13	Joback Method

cpg	333.56	J/mol×K	577.77	Joback Method
cpg	400.68	J/mol×K	774.59	Joback Method
dvisc	0.0007272	Pa×s	538.40	Joback Method
dvisc	0.0008027	Pa×s	504.22	Joback Method
dvisc	0.0008987	Pa×s	470.05	Joback Method
dvisc	0.0010242	Pa×s	435.87	Joback Method
dvisc	0.0011935	Pa×s	401.69	Joback Method
dvisc	0.0014309	Pa×s	367.52	Joback Method
dvisc	0.0017806	Pa×s	333.34	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1076171&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

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
ie: Ionization energy
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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