1H-Indene, 2,3-dihydro-1,1,4,6,7-pentamethyl

Inchi: InChI=1S/C14H20/c1-9-8-10(2)12-6-7-14(4,5)13(12)11(9)3/h8H,6-7H2,1-5H3
InchiKey: DKEQNICHDTZGAN-UHFFFAOYSA-N
Formula: C14H20
SMILES: Cc1cc(C)c2c(c1C)C(C)(C)CC2
Mol. weight [g/mol]: 188.31

Physical Properties

Property code	Value	Unit	Source
gf	196.15	kJ/mol	Joback Method
hf	-53.60	kJ/mol	Joback Method
hfus	16.34	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.836		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	573.30	K	Joback Method
tc	794.18	K	Joback Method
tf	365.88	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.27	J/mol×K	573.30	Joback Method
cpg	445.90	J/mol×K	610.11	Joback Method
cpg	462.52	J/mol×K	646.93	Joback Method
cpg	478.25	J/mol×K	683.74	Joback Method
cpg	493.24	J/mol×K	720.55	Joback Method
cpg	507.65	J/mol×K	757.36	Joback Method
cpg	521.60	J/mol×K	794.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R71153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume