1H-Indene, 2,3-dihydro-1,1,3,3,5-pentamethyl-

Other names: 1,1,3,3,5-pentamethylindan
Inchi: InChI=1S/C14H20/c1-10-6-7-11-12(8-10)14(4,5)9-13(11,2)3/h6-8H,9H2,1-5H3
InchiKey: NNXHDILUOAXSPU-UHFFFAOYSA-N
Formula: C14H20
SMILES: Cc1ccc2c(c1)C(C)(C)CC2(C)C
Mol. weight [g/mol]: 188.31
CAS: 81-03-8

Physical Properties

Property code	Value	Unit	Source
gf	202.21	kJ/mol	Joback Method
hf	-35.76	kJ/mol	Joback Method
hfus	11.89	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.954		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1259.00		NIST Webbook
tb	558.91	K	Joback Method
tc	786.68	K	Joback Method
tf	360.50	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.11	J/mol×K	558.91	Joback Method
cpg	446.66	J/mol×K	596.87	Joback Method
cpg	463.96	J/mol×K	634.83	Joback Method
cpg	480.26	J/mol×K	672.80	Joback Method
cpg	495.84	J/mol×K	710.76	Joback Method
cpg	510.94	J/mol×K	748.72	Joback Method
cpg	525.83	J/mol×K	786.68	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=C81038&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