1H-Indene, 2,3-dihydro-1,1,4,7-tetramethyl-

Other names: Indan, 1,1,4,7-tetramethyl-
1,1,4,7-Tetramethylindan
Inchi: InChI=1S/C13H18/c1-9-5-6-10(2)12-11(9)7-8-13(12,3)4/h5-6H,7-8H2,1-4H3
InchiKey: IFZVSOLCUIWLFW-UHFFFAOYSA-N
Formula: C13H18
SMILES: Cc1ccc(C)c2c1CCC2(C)C
Mol. weight [g/mol]: 174.28
CAS: 1078-04-2

Physical Properties

Property code	Value	Unit	Source
chl	-7564.20 ± 1.70	kJ/mol	NIST Webbook
gf	197.36	kJ/mol	Joback Method
hf	-62.50 ± 1.90	kJ/mol	NIST Webbook
hfl	-123.90 ± 1.80	kJ/mol	NIST Webbook
hfus	14.14	kJ/mol	Joback Method
hvap	61.40 ± 0.60	kJ/mol	NIST Webbook
hvap	61.37 ± 0.61	kJ/mol	NIST Webbook
log10ws	-4.02		Crippen Method
logp	3.527		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1333.00		NIST Webbook
sl	343.50	J/mol×K	NIST Webbook
tb	545.44	K	Joback Method
tc	769.28	K	Joback Method
tf	342.09	K	Joback Method
tt	245.55 ± 0.01	K	NIST Webbook
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.93	J/mol×K	769.28	Joback Method

cpg	397.09	J/mol×K	582.75	Joback Method
cpg	413.31	J/mol×K	620.05	Joback Method
cpg	428.55	J/mol×K	657.36	Joback Method
cpg	442.97	J/mol×K	694.67	Joback Method
cpg	456.71	J/mol×K	731.97	Joback Method
cpg	379.74	J/mol×K	545.44	Joback Method
cpl	302.50	J/mol×K	298.15	NIST Webbook
hfust	11.28	kJ/mol	245.55	NIST Webbook
hfust	11.28	kJ/mol	245.60	NIST Webbook
hvapt	59.60	kJ/mol	350.50	NIST Webbook
hvapt	60.40	kJ/mol	391.00	NIST Webbook
hvapt	52.00	kJ/mol	450.00	NIST Webbook

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=C1078042&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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

sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume