1H-Indene, 2,3-dihydro-1,1,3-trimethyl-

Other names: Indan, 1,1,3-trimethyl-
1,1,3-Trimethylindan
1,1,3-Trimethylindane
1,1,3-Trimethyl-(2,3-dihydroindene)
2,3-Dihydro-1,1,3-trimethyl-1H-indene
Indane, 1,1,3-trimethyl

Inchi: InChI=1S/C12H16/c1-9-8-12(2,3)11-7-5-4-6-10(9)11/h4-7,9H,8H2,1-3H3

InchiKey: CPLBLNGVYBSVPU-UHFFFAOYSA-N

Formula: C12H16

SMILES: CC1CC(C)(C)c2ccccc21

Mol. weight [g/mol]: 160.26

CAS: 2613-76-5

Physical Properties

Property code	Value	Unit	Source
gf	200.49	kJ/mol	Joback Method
hf	1.75	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	43.70	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.471		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1178.00		NIST Webbook
tb	507.93	K	Joback Method
tc	733.35	K	Joback Method
tf	301.54	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.97	J/mol×K	507.93	Joback Method
cpg	350.99	J/mol×K	545.50	Joback Method

cpg	367.68	J/mol×K	583.07	Joback Method
cpg	383.21	J/mol×K	620.64	Joback Method
cpg	397.73	J/mol×K	658.21	Joback Method
cpg	411.39	J/mol×K	695.78	Joback Method
cpg	424.37	J/mol×K	733.35	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2613765&Units=SI

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