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

Other names: Indan, 1,1,3-trimethyl-3-phenyl-
1-Phenyl-1,3,3-trimethylindan
1-Phenyl-1,3,3-trimethylindane
1,1,3-Trimethyl-3-phenylindan
1,1,3-Trimethyl-3-phenylindane
1,3,3-Trimethyl-1-phenylindan
2,3-Dihydro-1,1,3-trimethyl-3-phenyl-1H-indene
1,3,3-Trimethyl-1-phenylindane
NSC 11311
NSC 55135
Styrene, alpha-methyl-, dimer

Inchi: InChI=1S/C18H20/c1-17(2)13-18(3,14-9-5-4-6-10-14)16-12-8-7-11-15(16)17/h4-12H,13H

InchiKey: ICLPNZMYHDVKKI-UHFFFAOYSA-N

Formula: C18H20

SMILES: CC1(C)CC(C)(c2ccccc2)c2ccccc21

Mol. weight [g/mol]: 236.35

CAS: 3910-35-8

Physical Properties

Property code	Value	Unit	Source
gf	357.93	kJ/mol	Joback Method
hf	129.68	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.674		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	582.00 ± 5.00	K	NIST Webbook
tc	928.72	K	Joback Method
tf	326.00 ± 3.00	K	NIST Webbook
tf	325.00 ± 3.00	K	NIST Webbook
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.56	J/mol×K	672.13	Joback Method
cpg	577.81	J/mol×K	714.89	Joback Method
cpg	597.11	J/mol×K	757.66	Joback Method
cpg	615.89	J/mol×K	800.42	Joback Method
cpg	634.56	J/mol×K	843.19	Joback Method
cpg	653.55	J/mol×K	885.95	Joback Method
cpg	673.27	J/mol×K	928.72	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3910358&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

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