1H-Indene, 5-(1,1-dimethylethyl)-2,3-dihydro-1,1-dimethyl-

Other names: Indan, 5-tert-butyl-1,1-dimethyl-
5-(tert-butyl)-1,1-dimethylindan

Inchi: InChI=1S/C15H22/c1-14(2,3)12-6-7-13-11(10-12)8-9-15(13,4)5/h6-7,10H,8-9H2,1-5H3

InchiKey: CVJYZSZDNBCBSS-UHFFFAOYSA-N

Formula: C15H22

SMILES: CC(C)(C)c1ccc2c(c1)CCC2(C)C

Mol. weight [g/mol]: 202.34

CAS: 38393-97-4

Physical Properties

Property code	Value	Unit	Source
gf	226.67	kJ/mol	Joback Method
hf	-60.05	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	50.05	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.208		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
tb	582.99	K	Joback Method
tc	811.44	K	Joback Method
tf	354.53	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.16	J/mol×K	582.99	Joback Method
cpg	501.04	J/mol×K	621.07	Joback Method
cpg	519.55	J/mol×K	659.14	Joback Method
cpg	536.90	J/mol×K	697.22	Joback Method
cpg	553.27	J/mol×K	735.29	Joback Method
cpg	568.88	J/mol×K	773.37	Joback Method
cpg	583.93	J/mol×K	811.44	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=C38393974&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume