1H-Indene, 2,3,3a,4-tetrahydro-3,3a,6-trimethyl-1-(1-methyleth

Inchi: InChI=1S/C15H24/c1-10(2)13-9-12(4)15(5)7-6-11(3)8-14(13)15/h6,8,10,12-13H,7,9H2,1-

InchiKey: IVBZYUKCNLJUDA-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC1=CCC2(C)C(=C1)C(C(C)C)CC2C

Mol. weight [g/mol]: 204.35

CAS: 59742-39-1

Physical Properties

Property code	Value	Unit	Source
gf	185.64	kJ/mol	Joback Method
hf	-143.57	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	49.39	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	572.30	K	Joback Method
tc	788.72	K	Joback Method
tf	315.35	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.17	J/mol×K	572.30	Joback Method
cpg	521.79	J/mol×K	608.37	Joback Method
cpg	542.14	J/mol×K	644.44	Joback Method
cpg	561.33	J/mol×K	680.51	Joback Method
cpg	579.53	J/mol×K	716.58	Joback Method
cpg	596.86	J/mol×K	752.65	Joback Method
cpg	613.48	J/mol×K	788.72	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=C59742391&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