1H-Indene, 2,3-dihydro-1,1,5-trimethyl-

Other names: 1,1,5-Trimethylindan
2,3-Dihydro-1,1,5-trimethyl-1H-indene
Inchi: InChI=1S/C12H16/c1-9-4-5-11-10(8-9)6-7-12(11,2)3/h4-5,8H,6-7H2,1-3H3
InchiKey: JIHZHLCOASGNCG-UHFFFAOYSA-N
Formula: C12H16
SMILES: Cc1ccc2c(c1)CCC2(C)C
Mol. weight [g/mol]: 160.26
CAS: 40650-41-7

Physical Properties

Property code	Value	Unit	Source
gf	198.57	kJ/mol	Joback Method
hf	10.62	kJ/mol	Joback Method
hfus	11.94	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.219		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	225.74		NIST Webbook
tb	517.58	K	Joback Method
tc	744.34	K	Joback Method
tf	318.30	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.59	J/mol×K	517.58	Joback Method
cpg	349.69	J/mol×K	555.37	Joback Method
cpg	365.53	J/mol×K	593.17	Joback Method
cpg	380.29	J/mol×K	630.96	Joback Method
cpg	394.12	J/mol×K	668.75	Joback Method
cpg	407.20	J/mol×K	706.55	Joback Method

cpg	419.67	J/mol×K	744.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32644e+01
Coeff. B	-3.78101e+03
Coeff. C	-8.20230e+01
Temperature range (K), min.	373.39
Temperature range (K), max.	557.45

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C40650417&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
pvap: Vapor pressure
rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume