

1H-Indene, 2,3-dihydro-1,4,7-trimethyl-

Other names:	1,4,7-Trimethyl-(2,3-dihydroindene) 1,4,7-Trimethylindan 2,3-Dihydro-1,4,7-trimethyl-1H-indene
Inchi:	InChI=1S/C12H16/c1-8-4-5-9(2)12-10(3)6-7-11(8)12/h4-5,10H,6-7H2,1-3H3
InchiKey:	VPYDMFMIOKBZIO-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	<chem>Cc1ccc(C)c2c1CCC2C</chem>
Mol. weight [g/mol]:	160.26
CAS:	54340-87-3

Physical Properties

Property code	Value	Unit	Source
gf	194.43	kJ/mol	Joback Method
hf	-16.09	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.353		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	226.59		NIST Webbook
rinpol	1288.00		NIST Webbook
tb	522.32	K	Joback Method
tc	740.90	K	Joback Method
tf	306.92	K	Joback Method
vc	0.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.14	J/mol×K	522.32	Joback Method
cpg	349.98	J/mol×K	558.75	Joback Method
cpg	365.83	J/mol×K	595.18	Joback Method
cpg	380.73	J/mol×K	631.61	Joback Method

cpg	394.75	J/molxK	668.04	Joback Method
cpg	407.93	J/molxK	704.47	Joback Method
cpg	420.33	J/molxK	740.90	Joback Method
dvisc	0.0011556	Paxs	306.92	Joback Method
dvisc	0.0008783	Paxs	342.82	Joback Method
dvisc	0.0007032	Paxs	378.72	Joback Method
dvisc	0.0005851	Paxs	414.62	Joback Method
dvisc	0.0005013	Paxs	450.52	Joback Method
dvisc	0.0004395	Paxs	486.42	Joback Method
dvisc	0.0003923	Paxs	522.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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=C54340873&Units=SI
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/ci990307I

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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