1,2,3-Trimethylindene

Other names: 1H-Indene, 1,2,3-trimethyl-
Inchi: InChI=1S/C12H14/c1-8-9(2)11-6-4-5-7-12(11)10(8)3/h4-7,9H,1-3H3
InchiKey: NPXPQDMZVKFLKB-UHFFFAOYSA-N
Formula: C12H14
SMILES: CC1=C(C)C(C)c2ccccc21
Mol. weight [g/mol]: 158.24
CAS: 4773-83-5

Physical Properties

Property code	Value	Unit	Source
gf	224.39	kJ/mol	Joback Method
hf	41.69	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.597		Crippen Method
mcvol	141.020	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	521.48	K	Joback Method
tc	742.25	K	Joback Method
tf	307.68	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.37	J/mol×K	521.48	Joback Method
cpg	330.98	J/mol×K	558.28	Joback Method
cpg	345.63	J/mol×K	595.07	Joback Method
cpg	359.37	J/mol×K	631.87	Joback Method
cpg	372.26	J/mol×K	668.66	Joback Method
cpg	384.36	J/mol×K	705.46	Joback Method
cpg	395.71	J/mol×K	742.25	Joback Method
dvisc	0.0010063	Pa×s	307.68	Joback Method

dvisc	0.0007924	Pa×s	343.31	Joback Method
dvisc	0.0006527	Pa×s	378.95	Joback Method
dvisc	0.0005558	Pa×s	414.58	Joback Method
dvisc	0.0004855	Pa×s	450.21	Joback Method
dvisc	0.0004326	Pa×s	485.85	Joback Method
dvisc	0.0003915	Pa×s	521.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.83546e+01
Coeff. B	-7.38909e+03
Coeff. C	-3.08973e+00
Coeff. D	1.79554e-07
Temperature range (K), min.	344.65
Temperature range (K), max.	726.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4773835&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=779
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

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