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

Other names: Indan, 1,1,4-trimethyl-
1,1,4-Trimethylindan
Inchi: InChI=1S/C12H16/c1-9-5-4-6-11-10(9)7-8-12(11,2)3/h4-6H,7-8H2,1-3H3
InchiKey: USZSMCUXEWREKR-UHFFFAOYSA-N
Formula: C12H16
SMILES: Cc1cccc2c1CCC2(C)C
Mol. weight [g/mol]: 160.26
CAS: 16204-72-1

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
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

Sources

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=C16204721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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