

1H-INDENE, 1,1,3-TRIMETHYL-

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

Physical Properties

Property code	Value	Unit	Source
hfus	13.16	kJ/mol	Joback Method
ie	7.89	eV	Cheméo Relay (1.0)
logp	3.381		Crippen Method
mcvol	141.020	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.01	J/mol×K	516.74	Joback Method
cpg	330.83	J/mol×K	554.92	Joback Method
cpg	345.43	J/mol×K	593.11	Joback Method
cpg	358.97	J/mol×K	631.29	Joback Method
cpg	371.63	J/mol×K	669.47	Joback Method
cpg	383.58	J/mol×K	707.65	Joback Method
cpg	394.98	J/mol×K	745.84	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2177459&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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