

1H-Indene, 1-ethyl-2,3-dihydro-1-methyl-

Inchi:	InChI=1S/C12H16/c1-3-12(2)9-8-10-6-4-5-7-11(10)12/h4-7H,3,8-9H2,1-2H3
InchiKey:	PVWWWDUASYPYLN-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	CCC1(C)CCc2ccccc21
Mol. weight [g/mol]:	160.26
CAS:	56298-75-0

Physical Properties

Property code	Value	Unit	Source
gf	208.20	kJ/mol	Joback Method
hf	22.09	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.300		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	512.60	K	Joback Method
tc	738.14	K	Joback Method
tf	305.78	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.16	J/molxK	512.60	Joback Method
cpg	349.70	J/molxK	550.19	Joback Method
cpg	365.90	J/molxK	587.78	Joback Method
cpg	380.94	J/molxK	625.37	Joback Method
cpg	394.98	J/molxK	662.96	Joback Method
cpg	408.20	J/molxK	700.55	Joback Method
cpg	420.75	J/molxK	738.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56298750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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