

3a,7a-Ethano-1H-indene, hexahydro-

Inchi:	InChI=1S/C11H18/c1-2-5-11-7-3-6-10(11,4-1)8-9-11/h1-9H2
InchiKey:	FVWMSEVAVPABAY-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C1CCC2CCCC2(C1)CC3
Mol. weight [g/mol]:	150.26
CAS:	43043-80-7

Physical Properties

Property code	Value	Unit	Source
gf	196.52	kJ/mol	Joback Method
hf	-13.47	kJ/mol	Joback Method
hfus	0.78	kJ/mol	Joback Method
hvap	38.17	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.511		Crippen Method
mcvol	133.270	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	484.99	K	Joback Method
tc	724.65	K	Joback Method
tf	312.55	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.62	J/mol×K	484.99	Joback Method
cpg	342.94	J/mol×K	524.93	Joback Method
cpg	362.97	J/mol×K	564.88	Joback Method
cpg	381.09	J/mol×K	604.82	Joback Method
cpg	397.67	J/mol×K	644.76	Joback Method
cpg	413.10	J/mol×K	684.71	Joback Method
cpg	427.74	J/mol×K	724.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43043807&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
mccvol:	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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