

1,3-Hexadiene, 3-ethyl-2-methyl-

Other names:	3-Ethyl-2-methyl-1,3-hexadiene
Inchi:	InChI=1S/C9H16/c1-5-7-9(6-2)8(3)4/h7H,3,5-6H2,1-2,4H3/b9-7+
InchiKey:	ICVZMTIGTXBIHI-VQHVLOKHSA-N
Formula:	C9H16
SMILES:	C=C(C)C(=CCC)CC
Mol. weight [g/mol]:	124.22
CAS:	61142-36-7

Physical Properties

Property code	Value	Unit	Source
gf	175.86	kJ/mol	Joback Method
hf	-6.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1005.00		NIST Webbook
tb	405.92	K	Joback Method
tc	587.50	K	Joback Method
tf	156.43	K	Joback Method
vc	0.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.60	J/mol×K	405.92	Joback Method

cpg	256.52	J/mol×K	436.18	Joback Method
cpg	269.78	J/mol×K	466.45	Joback Method
cpg	282.41	J/mol×K	496.71	Joback Method
cpg	294.43	J/mol×K	526.98	Joback Method
cpg	305.86	J/mol×K	557.24	Joback Method
cpg	316.74	J/mol×K	587.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61142367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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