

(Z)-3-Hexene, 2,2-dimethyl

Inchi:	InChI=1S/C9H18/c1-5-6-7-8-9(2,3)4/h7-8H,5-6H2,1-4H3/b8-7-
InchiKey:	BQOCYCICSYUPRF-FPLPWBNLSA-N
Formula:	C9H18
SMILES:	CCCC=CC(C)(C)C
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	107.96	kJ/mol	Joback Method
hf	-120.62	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	34.29	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	723.00		NIST Webbook
rinpol	726.00		NIST Webbook
rinpol	724.00		NIST Webbook
tb	406.25	K	Joback Method
tc	588.59	K	Joback Method
tf	188.53	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.57	J/mol×K	406.25	Joback Method
cpg	329.51	J/mol×K	558.20	Joback Method
cpg	317.00	J/mol×K	527.81	Joback Method
cpg	303.79	J/mol×K	497.42	Joback Method
cpg	289.84	J/mol×K	467.03	Joback Method
cpg	275.11	J/mol×K	436.64	Joback Method
cpg	341.36	J/mol×K	588.59	Joback Method

dvisc	0.0002180	Pa×s	406.25	Joback Method
dvisc	0.0003038	Pa×s	369.96	Joback Method
dvisc	0.0004551	Pa×s	333.68	Joback Method
dvisc	0.0007523	Pa×s	297.39	Joback Method
dvisc	0.0014301	Pa×s	261.10	Joback Method
dvisc	0.0033453	Pa×s	224.82	Joback Method
dvisc	0.0108529	Pa×s	188.53	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=R42714&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
dvisc:	Dynamic viscosity
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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