

(Z)-3-Methyl-2-octene

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

Physical Properties

Property code	Value	Unit	Source
gf	102.68	kJ/mol	Joback Method
hf	-117.15	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	35.20	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	907.00		NIST Webbook
tb	409.04	K	Joback Method
tc	584.08	K	Joback Method
tf	171.11	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.03	J/mol×K	409.04	Joback Method
cpg	272.42	J/mol×K	438.21	Joback Method
cpg	286.19	J/mol×K	467.39	Joback Method
cpg	299.36	J/mol×K	496.56	Joback Method
cpg	311.95	J/mol×K	525.73	Joback Method
cpg	323.98	J/mol×K	554.90	Joback Method
cpg	335.48	J/mol×K	584.08	Joback Method
dvisc	0.0104021	Pa×s	171.11	Joback Method
dvisc	0.0028673	Pa×s	210.77	Joback Method

dvisc	0.0011887	Pa×s	250.42	Joback Method
dvisc	0.0006269	Pa×s	290.07	Joback Method
dvisc	0.0003857	Pa×s	329.73	Joback Method
dvisc	0.0002633	Pa×s	369.38	Joback Method
dvisc	0.0001936	Pa×s	409.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R108571&Units=SI

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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