

2-Methyloct-4-ene

Other names:	2-methyl-4-octene
Inchi:	InChI=1S/C9H18/c1-4-5-6-7-8-9(2)3/h6-7,9H,4-5,8H2,1-3H3/b7-6+
InchiKey:	IGMJZWHHNPRADN-VOTSOKGWSA-N
Formula:	C9H18
SMILES:	CCCC=CCC(C)C
Mol. weight [g/mol]:	126.24
CAS:	64501-77-5

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	887.00		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/molxK	409.04	Joback Method
cpg	323.98	J/molxK	554.90	Joback Method
cpg	311.95	J/molxK	525.73	Joback Method
cpg	299.36	J/molxK	496.56	Joback Method
cpg	286.19	J/molxK	467.39	Joback Method
cpg	272.42	J/molxK	438.21	Joback Method
cpg	335.48	J/molxK	584.08	Joback Method

dvisc	0.0001936	Paxs	409.04	Joback Method
dvisc	0.0002633	Paxs	369.38	Joback Method
dvisc	0.0003857	Paxs	329.73	Joback Method
dvisc	0.0006269	Paxs	290.07	Joback Method
dvisc	0.0011887	Paxs	250.42	Joback Method
dvisc	0.0028673	Paxs	210.77	Joback Method
dvisc	0.0104021	Paxs	171.11	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44881e+01
Coeff. B	-3.57130e+03
Coeff. C	-5.57280e+01
Temperature range (K), min.	307.22
Temperature range (K), max.	444.90

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64501775&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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

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