1-Octene, 6-methyl-

Other names: 6-Methyl-1-octene
Inchi: InChI=1S/C9H18/c1-4-6-7-8-9(3)5-2/h4,9H,1,5-8H2,2-3H3
InchiKey: NFTYCFXCGQYTKV-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=CCCCC(C)CC
Mol. weight [g/mol]: 126.24
CAS: 13151-10-5

Physical Properties

Property code	Value	Unit	Source
gf	110.30	kJ/mol	Joback Method
hf	-108.94	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	34.57	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
tb	401.56	K	Joback Method
tc	571.62	K	Joback Method
tf	174.43	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.23	J/mol×K	401.56	Joback Method
cpg	321.86	J/mol×K	543.28	Joback Method
cpg	309.99	J/mol×K	514.93	Joback Method

cpg	297.60	J/mol×K	486.59	Joback Method
cpg	284.69	J/mol×K	458.25	Joback Method
cpg	271.24	J/mol×K	429.90	Joback Method
cpg	333.24	J/mol×K	571.62	Joback Method
dvisc	0.0002302	Pa×s	401.56	Joback Method
dvisc	0.0003086	Pa×s	363.70	Joback Method
dvisc	0.0004428	Pa×s	325.85	Joback Method
dvisc	0.0006987	Pa×s	288.00	Joback Method
dvisc	0.0012657	Pa×s	250.14	Joback Method
dvisc	0.0028336	Pa×s	212.28	Joback Method
dvisc	0.0090007	Pa×s	174.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59744e+01
Coeff. B	-4.07439e+03
Coeff. C	-5.87860e+01
Temperature range (K), min.	318.52
Temperature range (K), max.	440.90

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13151105&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume