1-OCTENE, 3-METHYL-

Other names: 3-Methyl-1-octene
Inchi: InChI=1S/C9H18/c1-4-6-7-8-9(3)5-2/h5,9H,2,4,6-8H2,1,3H3
InchiKey: GLUPFQMLFXGTNL-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=CC(C)CCCCC
Mol. weight [g/mol]: 126.24
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.3508		Cheméo Relay (1.0)
gf	110.30	kJ/mol	Joback Method
hf	-125.78	kJ/mol	Cheméo Relay (1.0)
hfus	14.26	kJ/mol	Joback Method
hvap	41.11	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-4.88		Cheméo Relay (1.0)
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	840.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	840.00		NIST Webbook
tb	411.39 ± 0.40	K	NIST Webbook
tb	409.50 ± 1.50	K	NIST Webbook
tc	565.69	K	Cheméo Relay (1.0)
tf	181.07	K	Cheméo Relay (1.0)
vc	0.496	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.23	J/mol×K	401.56	Joback Method
cpg	271.24	J/mol×K	429.90	Joback Method
cpg	284.69	J/mol×K	458.25	Joback Method
cpg	297.60	J/mol×K	486.59	Joback Method
cpg	309.99	J/mol×K	514.93	Joback Method
cpg	321.86	J/mol×K	543.28	Joback Method
cpg	333.24	J/mol×K	571.62	Joback Method
dvisc	0.0090007	Pa×s	174.43	Joback Method
dvisc	0.0028336	Pa×s	212.28	Joback Method
dvisc	0.0012657	Pa×s	250.14	Joback Method
dvisc	0.0006987	Pa×s	288.00	Joback Method
dvisc	0.0004428	Pa×s	325.85	Joback Method
dvisc	0.0003086	Pa×s	363.70	Joback Method
dvisc	0.0002302	Pa×s	401.56	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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13151081&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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