1-Octene, 2-methyl-

Other names: 2-METHYLOCT-1-ENE
2-Methyl-1-octene
Inchi: InChI=1S/C9H18/c1-4-5-6-7-8-9(2)3/h2,4-8H2,1,3H3
InchiKey: FBEDQPGLIKZGIN-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=C(C)CCCCCC
Mol. weight [g/mol]: 126.24
CAS: 4588-18-5

Physical Properties

Property code	Value	Unit	Source
gf	104.19	kJ/mol	Joback Method
hf	-113.45	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	860.00		NIST Webbook

rinpol	880.00		NIST Webbook
tb	415.00 ± 5.00	K	NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	416.30 ± 2.00	K	NIST Webbook
tb	418.00 ± 0.20	K	NIST Webbook
tb	417.61 ± 0.30	K	NIST Webbook
tb	417.95 ± 0.25	K	NIST Webbook
tc	571.36	K	Joback Method
tf	195.29 ± 0.20	K	NIST Webbook
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.27	J/mol×K	401.88	Joback Method
cpg	271.11	J/mol×K	430.13	Joback Method
cpg	284.40	J/mol×K	458.37	Joback Method
cpg	297.17	J/mol×K	486.62	Joback Method
cpg	309.42	J/mol×K	514.87	Joback Method
cpg	321.16	J/mol×K	543.11	Joback Method
cpg	332.43	J/mol×K	571.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44084e+01
Coeff. B	-3.55904e+03
Coeff. C	-5.34660e+01
Temperature range (K), min.	305.51
Temperature range (K), max.	444.70

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4588185&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol342.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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