4-methyl-2-octene

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

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	842.00		NIST Webbook
rinpol	842.00		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	323.98	J/mol×K	554.90	Joback Method
cpg	311.95	J/mol×K	525.73	Joback Method
cpg	299.36	J/mol×K	496.56	Joback Method
cpg	286.19	J/mol×K	467.39	Joback Method
cpg	272.42	J/mol×K	438.21	Joback Method
cpg	335.48	J/mol×K	584.08	Joback Method

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

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=R141449&Units=SI

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

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