3-Heptene, 2,6-dimethyl-

Other names:	2,6-Dimethyl-3-heptene
	2,6-Dimethyl-3-heptene,c&t
	2,6-dimethylhept-3-ene
Inchi:	InChI=1S/C9H18/c1-8(2)6-5-7-9(3)4/h5-6,8-9H,7H2,1-4H3/b6-5+
InchiKey:	KDISTZUHDQPXDE-AATRIKPKSA-N
Formula:	C9H18
SMILES:	CC(C)C=CCC(C)C
Mol. weight [g/mol]:	126.24
CAS:	2738-18-3

Physical Properties

Property code	Value	Unit	Source
gf	100.24	kJ/mol	Joback Method
hf	-122.43	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	34.81	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	815.00		NIST Webbook
tb	387.40 ± 2.00	K	NIST Webbook
tc	587.67	K	Joback Method
tf	156.11	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.97	J/mol×K	408.60	Joback Method
cpg	272.79	J/mol×K	438.45	Joback Method
cpg	286.94	J/mol×K	468.29	Joback Method

cpg	300.46	J/mol×K	498.14	Joback Method
cpg	313.37	J/mol×K	527.98	Joback Method
cpg	325.70	J/mol×K	557.83	Joback Method
cpg	337.45	J/mol×K	587.67	Joback Method
dvisc	0.0223846	Pa×s	156.11	Joback Method
dvisc	0.0043187	Pa×s	198.19	Joback Method
dvisc	0.0014827	Pa×s	240.27	Joback Method
dvisc	0.0007001	Pa×s	282.36	Joback Method
dvisc	0.0004016	Pa×s	324.44	Joback Method
dvisc	0.0002618	Pa×s	366.52	Joback Method
dvisc	0.0001863	Pa×s	408.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57806e+01
Coeff. B	-3.75606e+03
Coeff. C	-5.09040e+01
Temperature range (K), min.	293.34
Temperature range (K), max.	409.68

Sources

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=C2738183&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

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