2,6-Octadiene

Other names: 1,6-DIMETHYLDIALLYL
Octa-2,6-diene
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-6H,7-8H2,1-2H3
InchiKey: LAGGTOBQMQHXON-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC=CCCC=CC
Mol. weight [g/mol]: 110.20
CAS: 4974-27-0

Physical Properties

Property code	Value	Unit	Source
gf	176.92	kJ/mol	Joback Method
hf	25.99	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	33.32	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	397.65 ± 0.50	K	NIST Webbook
tb	397.70 ± 1.00	K	NIST Webbook
tb	398.00 ± 1.00	K	NIST Webbook
tc	571.58	K	Joback Method
tf	169.76	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.62	J/mol×K	390.76	Joback Method
cpg	216.35	J/mol×K	420.90	Joback Method
cpg	228.43	J/mol×K	451.03	Joback Method
cpg	239.90	J/mol×K	481.17	Joback Method
cpg	250.79	J/mol×K	511.30	Joback Method

cpg	261.13	J/mol×K	541.44	Joback Method
cpg	270.94	J/mol×K	571.58	Joback Method
dvisc	0.0049045	Pa×s	169.76	Joback Method
dvisc	0.0016869	Pa×s	206.59	Joback Method
dvisc	0.0008014	Pa×s	243.43	Joback Method
dvisc	0.0004630	Pa×s	280.26	Joback Method
dvisc	0.0003039	Pa×s	317.09	Joback Method
dvisc	0.0002177	Pa×s	353.93	Joback Method
dvisc	0.0001661	Pa×s	390.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53464e+01
Coeff. B	-3.73343e+03
Coeff. C	-5.16970e+01
Temperature range (K), min.	299.62
Temperature range (K), max.	423.74

Sources

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=391

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4974270&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume