2,6-Octadiene, 4-methyl-

Other names: 4-methyl-2,6-octadiene
Inchi: InChI=1S/C9H16/c1-4-6-8-9(3)7-5-2/h4-7,9H,8H2,1-3H3/b6-4+,7-5+
InchiKey: UVAJNHJZOQGXLA-YDFGWWAZSA-N
Formula: C9H16
SMILES: CC=CCC(C)C=CC
Mol. weight [g/mol]: 124.22
CAS: 74498-94-5

Physical Properties

Property code	Value	Unit	Source
gf	182.90	kJ/mol	Joback Method
hf	0.07	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	35.16	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	413.20	K	Joback Method
tc	597.12	K	Joback Method
tf	166.03	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.24	J/mol×K	413.20	Joback Method
cpg	307.48	J/mol×K	566.47	Joback Method
cpg	295.94	J/mol×K	535.81	Joback Method
cpg	283.78	J/mol×K	505.16	Joback Method
cpg	270.96	J/mol×K	474.51	Joback Method
cpg	257.46	J/mol×K	443.85	Joback Method
cpg	318.43	J/mol×K	597.12	Joback Method
dvisc	0.0001604	Pa×s	413.20	Joback Method

dvisc	0.0002181	Pa×s	372.00	Joback Method
dvisc	0.0003204	Pa×s	330.81	Joback Method
dvisc	0.0005249	Pa×s	289.62	Joback Method
dvisc	0.0010129	Pa×s	248.42	Joback Method
dvisc	0.0025386	Pa×s	207.22	Joback Method
dvisc	0.0100379	Pa×s	166.03	Joback Method

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=C74498945&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume