1,5-Heptadiene, 2,6-dimethyl-

Other names: 2,6-Dimethyl-1,5-heptadiene
2,6-dimethylhepta-1,5-diene
Inchi: InChI=1S/C9H16/c1-8(2)6-5-7-9(3)4/h7H,1,5-6H2,2-4H3
InchiKey: DONSTYDPUORSDN-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=C(C)CCC=C(C)C
Mol. weight [g/mol]: 124.22
CAS: 6709-39-3

Physical Properties

Property code	Value	Unit	Source
gf	175.86	kJ/mol	Joback Method
hf	-6.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	882.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	829.00		NIST Webbook
tb	415.10 ± 2.00	K	NIST Webbook
tb	416.00 ± 2.00	K	NIST Webbook
tc	587.50	K	Joback Method
tf	170.50 ± 2.00	K	NIST Webbook
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.60	J/mol×K	405.92	Joback Method
cpg	256.52	J/mol×K	436.18	Joback Method
cpg	269.78	J/mol×K	466.45	Joback Method

cpg	282.41	J/mol×K	496.71	Joback Method
cpg	294.43	J/mol×K	526.98	Joback Method
cpg	305.86	J/mol×K	557.24	Joback Method
cpg	316.74	J/mol×K	587.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47786e+01
Coeff. B	-3.73259e+03
Coeff. C	-5.68400e+01
Temperature range (K), min.	314.42
Temperature range (K), max.	451.11

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol395.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6709393&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

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