1-Pentene, 3,4-dimethyl-

Other names: (CH3)2CHCH(CH3)CH=CH2
3,4-Dimethyl-1-pentene
Inchi: InChI=1S/C7H14/c1-5-7(4)6(2)3/h5-7H,1H2,2-4H3
InchiKey: WFHXQNMTMDKVJG-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=CC(C)C(C)C
Mol. weight [g/mol]: 98.19
CAS: 7385-78-6

Physical Properties

Property code	Value	Unit	Source
gf	91.02	kJ/mol	Joback Method
hf	-72.94	kJ/mol	Joback Method
hfus	5.56	kJ/mol	Joback Method
hvap	33.90	kJ/mol	NIST Webbook
log10ws	-2.12		Crippen Method
logp	2.465		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	636.80		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	641.30		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	637.20		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	641.30		NIST Webbook
rinpol	634.60		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	644.20		NIST Webbook
rinpol	646.40		NIST Webbook
rinpol	637.20		NIST Webbook
rinpol	639.50		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	647.00		NIST Webbook

rinpol	637.30		NIST Webbook
rinpol	637.80		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	644.40		NIST Webbook
rinpol	636.40		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	636.40		NIST Webbook
tb	353.95 ± 1.00	K	NIST Webbook
tb	363.05	K	NIST Webbook
tb	353.93 ± 0.30	K	NIST Webbook
tb	353.96 ± 0.20	K	NIST Webbook
tc	530.42	K	Joback Method
tf	136.89	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.12	J/mol×K	530.42	Joback Method
cpg	235.41	J/mol×K	501.24	Joback Method
cpg	225.27	J/mol×K	472.06	Joback Method
cpg	214.68	J/mol×K	442.89	Joback Method
cpg	203.64	J/mol×K	413.71	Joback Method
cpg	192.13	J/mol×K	384.54	Joback Method
cpg	180.13	J/mol×K	355.36	Joback Method
dvisc	0.0179569	Pa×s	136.89	Joback Method
dvisc	0.0002201	Pa×s	355.36	Joback Method
dvisc	0.0003016	Pa×s	318.95	Joback Method
dvisc	0.0004481	Pa×s	282.54	Joback Method
dvisc	0.0007487	Pa×s	246.13	Joback Method
dvisc	0.0014946	Pa×s	209.71	Joback Method
dvisc	0.0039899	Pa×s	173.30	Joback Method

hvapt	33.20	kJ/mol	343.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37935e+01
Coeff. B	-2.74141e+03
Coeff. C	-5.51640e+01
Temperature range (K), min.	258.14
Temperature range (K), max.	378.37

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=238
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7385786&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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