1-Pentene, 3,3-dimethyl-

Other names: 3,3-Dimethyl-1-pentene
3,3-dimethylpent-1-ene
Inchi: InChI=1S/C7H14/c1-5-7(3,4)6-2/h5H,1,6H2,2-4H3
InchiKey: TXBZITDWMURSEF-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=CC(C)(C)CC
Mol. weight [g/mol]: 98.19
CAS: 3404-73-7

Physical Properties

Property code	Value	Unit	Source
gf	98.74	kJ/mol	Joback Method
hf	-71.13	kJ/mol	Joback Method
hfus	5.19	kJ/mol	Joback Method
hvap	33.50	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	617.00		NIST Webbook
rinpol	623.70		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	631.60		NIST Webbook
rinpol	633.80		NIST Webbook
rinpol	626.40		NIST Webbook
rinpol	628.80		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	628.40		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	629.00		NIST Webbook

rinpol	626.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	630.10		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	632.80		NIST Webbook
rinpol	624.80		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	632.00		NIST Webbook
tb	350.05 ± 0.50	K	NIST Webbook
tb	350.69 ± 0.30	K	NIST Webbook
tb	350.70 ± 0.40	K	NIST Webbook
tb	350.69 ± 0.30	K	NIST Webbook
tb	350.05 ± 0.60	K	NIST Webbook
tb	350.05 ± 0.60	K	NIST Webbook
tb	350.70	K	NIST Webbook
tb	350.25 ± 0.50	K	NIST Webbook
tc	531.33	K	Joback Method
tf	138.77 ± 0.02	K	NIST Webbook
tf	138.74 ± 0.04	K	NIST Webbook
tf	138.74 ± 0.03	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.87	J/mol×K	353.01	Joback Method
cpg	193.78	J/mol×K	382.73	Joback Method
cpg	206.04	J/mol×K	412.45	Joback Method
cpg	217.68	J/mol×K	442.17	Joback Method
cpg	228.72	J/mol×K	471.89	Joback Method
cpg	239.19	J/mol×K	501.61	Joback Method

cpg	249.12	J/mol×K	531.33	Joback Method
dvisc	0.0092538	Pa×s	169.31	Joback Method
dvisc	0.0032853	Pa×s	199.93	Joback Method
dvisc	0.0015356	Pa×s	230.54	Joback Method
dvisc	0.0008579	Pa×s	261.16	Joback Method
dvisc	0.0005415	Pa×s	291.78	Joback Method
dvisc	0.0003731	Pa×s	322.39	Joback Method
dvisc	0.0002742	Pa×s	353.01	Joback Method
hvapt	33.00	kJ/mol	340.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35929e+01
Coeff. B	-2.62548e+03
Coeff. C	-5.80820e+01
Temperature range (K), min.	255.41
Temperature range (K), max.	375.12

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/files/research/kdb/mol/mol237.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404737&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
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