2-Pentene, 2,4-dimethyl-

Other names: (CH3)2CHCH=C(CH3)2
2,4-Dimethyl-2-pentene
2,4-dimethylpent-2-ene
Inchi: InChI=1S/C7H14/c1-6(2)5-7(3)4/h5-6H,1-4H3
InchiKey: VVCFYASOGFVJFN-UHFFFAOYSA-N
Formula: C7H14
SMILES: CC(C)=CC(C)C
Mol. weight [g/mol]: 98.19
CAS: 625-65-0

Physical Properties

Property code	Value	Unit	Source
affp	812.00	kJ/mol	NIST Webbook
basg	783.10	kJ/mol	NIST Webbook
chl	-4632.27 ± 0.84	kJ/mol	NIST Webbook
gf	77.29	kJ/mol	Joback Method
hf	-85.66	kJ/mol	Joback Method
hfus	9.25	kJ/mol	Joback Method
hvap	34.30	kJ/mol	NIST Webbook
hvap	34.30	kJ/mol	NIST Webbook
hvap	34.50 ± 1.50	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	640.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.70		NIST Webbook
rinpol	643.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook

rinpol	655.50		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	649.00		NIST Webbook
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rinpol	655.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	655.50		NIST Webbook
rinpol	640.30		NIST Webbook
rinpol	640.70		NIST Webbook
rinpol	648.40		NIST Webbook
rinpol	649.10		NIST Webbook
rinpol	641.20		NIST Webbook
rinpol	654.90		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	654.00		NIST Webbook
tb	363.16	K	Joback Method
tc	543.24	K	Joback Method
tf	145.85 ± 0.05	K	NIST Webbook
tf	145.45 ± 0.01	K	NIST Webbook
tf	145.42 ± 0.02	K	NIST Webbook
tf	145.41 ± 0.03	K	NIST Webbook
tf	145.45 ± 0.02	K	NIST Webbook
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.38	J/mol×K	453.20	Joback Method
cpg	226.07	J/mol×K	483.22	Joback Method
cpg	236.27	J/mol×K	513.23	Joback Method
cpg	180.18	J/mol×K	363.16	Joback Method
cpg	192.45	J/mol×K	393.17	Joback Method
cpg	204.18	J/mol×K	423.19	Joback Method
cpg	246.01	J/mol×K	543.24	Joback Method
hvapt	35.20 ± 1.50	kJ/mol	286.50	NIST Webbook

hvapt	34.50	kJ/mol	324.50	NIST Webbook
hvapt	34.20	kJ/mol	324.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37580e+01
Coeff. B	-2.74151e+03
Coeff. C	-5.64900e+01
Temperature range (K), min.	260.01
Temperature range (K), max.	381.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.01167e+02
Coeff. B	-7.43140e+03
Coeff. C	-1.31513e+01
Coeff. D	1.24302e-05
Temperature range (K), min.	260.15
Temperature range (K), max.	380.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=242

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/mol242.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625650&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
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