1-Pentene, 2,4-dimethyl-

Other names: (CH3)2CHCH2C(CH3)=CH2
2,4-Dimethyl-1-pentene
2,4-dimethylpent-1-ene
Inchi: InChI=1S/C7H14/c1-6(2)5-7(3)4/h7H,1,5H2,2-4H3
InchiKey: LXQPBCHJNIOMQU-UHFFFAOYSA-N
Formula: C7H14
SMILES: C=C(C)CC(C)C
Mol. weight [g/mol]: 98.19
CAS: 2213-32-3

Physical Properties

Property code	Value	Unit	Source
chl	-4638.30 ± 1.70	kJ/mol	NIST Webbook
gf	84.91	kJ/mol	Joback Method
hf	-77.45	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	33.10	kJ/mol	NIST Webbook
hvap	33.10	kJ/mol	NIST Webbook
ie	9.03 ± 0.01	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	636.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	639.80		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	637.50		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	646.60		NIST Webbook

rinpol	656.00		NIST Webbook
rinpol	648.10		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	636.90		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	643.00		NIST Webbook
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rinpol	642.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	639.20		NIST Webbook
rinpol	637.90		NIST Webbook
rinpol	645.30		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	636.20		NIST Webbook
rinpol	646.50		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	645.90		NIST Webbook
ripol	734.00		NIST Webbook
tb	355.68	K	Joback Method
tc	530.11	K	Joback Method
tf	149.17 ± 0.50	K	NIST Webbook
tf	149.06 ± 0.06	K	NIST Webbook
tf	149.06 ± 0.04	K	NIST Webbook
tf	149.09 ± 0.02	K	NIST Webbook
tf	148.95 ± 0.50	K	NIST Webbook
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.34	J/mol×K	355.68	Joback Method
cpg	192.16	J/mol×K	384.75	Joback Method
cpg	203.51	J/mol×K	413.82	Joback Method
cpg	214.40	J/mol×K	442.89	Joback Method
cpg	224.84	J/mol×K	471.96	Joback Method
cpg	234.84	J/mol×K	501.04	Joback Method
cpg	244.42	J/mol×K	530.11	Joback Method
hvapt	32.30	kJ/mol	336.00	NIST Webbook
hvapt	33.20	kJ/mol	322.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39574e+01
Coeff. B	-2.86746e+03
Coeff. C	-4.77230e+01
Temperature range (K), min.	257.49
Temperature range (K), max.	379.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.26910e+01
Coeff. B	-6.60401e+03
Coeff. C	-1.03271e+01
Coeff. D	9.35835e-06
Temperature range (K), min.	289.15
Temperature range (K), max.	355.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol236.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2213323&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=236
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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