Pentane, 2,3,3,4-tetramethyl-

Other names: 2,3,3,4-Tetramethylpentane
Inchi: InChI=1S/C9H20/c1-7(2)9(5,6)8(3)4/h7-8H,1-6H3
InchiKey: JLCYYQOQSAMWTA-UHFFFAOYSA-N
Formula: C9H20
SMILES: CC(C)C(C)(C)C(C)C
Mol. weight [g/mol]: 128.26
CAS: 16747-38-9

Physical Properties

Property code	Value	Unit	Source
af	0.3130		KDB
chl	-6121.90 ± 1.60	kJ/mol	NIST Webbook
gf	34.12	kJ/mol	KDB
hcg	6121.95	kJ/mol	KDB
hcn	5681.830	kJ/mol	KDB
hf	-236.40	kJ/mol	KDB
hfus	4.61	kJ/mol	Joback Method
hvap	41.80	kJ/mol	NIST Webbook
log10ws	-2.86		Crippen Method
logp	3.325		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2716.00 ± 20.00	kPa	NIST Webbook
pc	2720.00	kPa	KDB
pc	2720.00 ± 40.00	kPa	NIST Webbook
rinpol	864.20		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	858.90		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	857.90		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	861.00		NIST Webbook

rinpol	858.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	860.90		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	854.70		NIST Webbook
rinpol	854.50		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	861.10		NIST Webbook
tb	414.55 ± 0.50	K	NIST Webbook
tb	414.69 ± 0.20	K	NIST Webbook
tb	414.72	K	KDB
tb	414.70	K	NIST Webbook
tb	414.70 ± 0.03	K	NIST Webbook
tb	414.55 ± 0.40	K	NIST Webbook
tb	414.35 ± 0.50	K	NIST Webbook
tb	414.69 ± 0.10	K	NIST Webbook
tb	405.00 ± 1.50	K	NIST Webbook
tc	607.50 ± 0.50	K	NIST Webbook
tc	607.50	K	KDB
tc	607.55 ± 0.20	K	NIST Webbook
tf	171.02 ± 0.05	K	NIST Webbook
tf	171.02 ± 0.02	K	NIST Webbook
tf	171.01 ± 0.10	K	NIST Webbook
tf	171.00	K	KDB
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.79	J/mol×K	401.21	Joback Method
cpg	290.35	J/mol×K	431.48	Joback Method
cpg	306.13	J/mol×K	461.76	Joback Method
cpg	321.15	J/mol×K	492.03	Joback Method
cpg	335.44	J/mol×K	522.31	Joback Method
cpg	349.03	J/mol×K	552.58	Joback Method
cpg	361.94	J/mol×K	582.85	Joback Method
dvisc	0.0002468	Pa×s	401.21	Joback Method
dvisc	0.0088523	Pa×s	203.21	Joback Method

dvisc	0.0512340	Pa×s	163.61	Joback Method
dvisc	0.0011576	Pa×s	282.41	Joback Method
dvisc	0.0006093	Pa×s	322.01	Joback Method
dvisc	0.0003691	Pa×s	361.61	Joback Method
dvisc	0.0027119	Pa×s	242.81	Joback Method
hvapt	34.94	kJ/mol	414.70	KDB
hvapt	39.30	kJ/mol	373.50	NIST Webbook
rfi	1.42003		298.15	KDB
rhol	755.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40767e+01
Coeff. B	-3.41898e+03
Coeff. C	-5.32210e+01
Temperature range (K), min.	301.17
Temperature range (K), max.	443.29

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.24133e+01
Coeff. B	-7.67624e+03
Coeff. C	-1.00145e+01
Coeff. D	6.27762e-06
Temperature range (K), min.	300.15
Temperature range (K), max.	607.50

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747389&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=97

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/mol97.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume