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

Other names: 2,2,3,3-Tetramethylpentane
Inchi: InChI=1S/C9H20/c1-7-9(5,6)8(2,3)4/h7H2,1-6H3
InchiKey: QUKOJKFJIHSBKV-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCC(C)(C)C(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 7154-79-2

Physical Properties

Property code	Value	Unit	Source
af	0.3030		KDB
ap	341.150	K	KDB
chl	-6121.60 ± 1.50	kJ/mol	NIST Webbook
gf	34.33	kJ/mol	KDB
hcg	6121.61	kJ/mol	KDB
hcn	5681.496	kJ/mol	KDB
hf	-237.40	kJ/mol	KDB
hfus	4.24	kJ/mol	Joback Method
hvap	41.20	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2740.00 ± 40.00	kPa	NIST Webbook
pc	2740.00	kPa	KDB
pc	2741.00 ± 20.00	kPa	NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	851.70		NIST Webbook
rinpol	857.10		NIST Webbook
rinpol	847.70		NIST Webbook

rinpol	847.80		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	855.80		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	852.70		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	855.00		NIST Webbook
sl	334.80	J/mol×K	NIST Webbook
tb	413.39 ± 0.20	K	NIST Webbook
tb	413.41 ± 0.10	K	NIST Webbook
tb	413.42 ± 0.03	K	NIST Webbook
tb	413.44	K	KDB
tb	413.50	K	NIST Webbook
tb	413.42 ± 0.20	K	NIST Webbook
tb	413.40 ± 0.40	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	263.11 ± 0.10	K	NIST Webbook
tf	263.30	K	KDB
tf	263.15 ± 0.50	K	NIST Webbook
tf	261.52 ± 0.20	K	NIST Webbook
tf	263.25 ± 0.10	K	NIST Webbook
tf	263.25 ± 0.08	K	NIST Webbook
tf	263.15 ± 0.30	K	NIST Webbook
tt	263.40 ± 0.02	K	NIST Webbook
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.90	J/mol×K	553.03	Joback Method
cpg	365.94	J/mol×K	583.86	Joback Method
cpg	275.15	J/mol×K	398.86	Joback Method
cpg	292.52	J/mol×K	429.69	Joback Method

cpg	308.94	J/mol×K	460.53	Joback Method
cpg	324.44	J/mol×K	491.36	Joback Method
cpg	339.09	J/mol×K	522.19	Joback Method
cpl	271.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0002923	Pa×s	398.86	Joback Method
dvisc	0.0024048	Pa×s	263.64	Joback Method
dvisc	0.0060005	Pa×s	229.84	Joback Method
dvisc	0.0205234	Pa×s	196.03	Joback Method
dvisc	0.0004276	Pa×s	365.06	Joback Method
dvisc	0.0006761	Pa×s	331.25	Joback Method
dvisc	0.0011864	Pa×s	297.44	Joback Method
hfust	2.33	kJ/mol	263.40	NIST Webbook
hfust	2.33	kJ/mol	263.40	NIST Webbook
hfust	7.33	kJ/mol	174.50	NIST Webbook
hvapt	35.27	kJ/mol	413.40	KDB
hvapt	39.20	kJ/mol	371.50	NIST Webbook
rfi	1.42140		298.15	KDB
rhol	757.00	kg/m3	293.00	KDB
sfust	8.90	J/mol×K	263.40	NIST Webbook
sfust	42.00	J/mol×K	174.50	NIST Webbook
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39261e+01
Coeff. B	-3.35151e+03
Coeff. C	-5.33610e+01
Temperature range (K), min.	299.10
Temperature range (K), max.	442.41

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.97422e+01
Coeff. B	-7.54526e+03
Coeff. C	-9.60312e+00
Coeff. D	5.74899e-06

Temperature range (K), min.	263.26
Temperature range (K), max.	610.85

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/mol94.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7154792&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=94
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density

rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume