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

Other names: 2,2,3,4-Tetramethylpentane
Inchi: InChI=1S/C9H20/c1-7(2)8(3)9(4,5)6/h7-8H,1-6H3
InchiKey: VZFMYOCAEQDWDY-UHFFFAOYSA-N
Formula: C9H20
SMILES: CC(C)C(C)C(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 1186-53-4

Physical Properties

Property code	Value	Unit	Source
af	0.3130		KDB
chl	-6122.20 ± 1.20	kJ/mol	NIST Webbook
gf	32.66	kJ/mol	KDB
hcg	6122.20	kJ/mol	KDB
hcn	5682.082	kJ/mol	KDB
hf	-237.10	kJ/mol	KDB
hfus	4.61	kJ/mol	Joback Method
hvap	40.80	kJ/mol	NIST Webbook
log10ws	-2.86		Crippen Method
logp	3.325		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2600.00 ± 40.00	kPa	NIST Webbook
pc	2602.00 ± 20.00	kPa	NIST Webbook
pc	2600.00	kPa	KDB
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	819.40		NIST Webbook
rinpol	824.80		NIST Webbook
rinpol	819.90		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	827.80		NIST Webbook
rinpol	827.80		NIST Webbook
rinpol	828.30		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	821.90		NIST Webbook
rinpol	820.00		NIST Webbook

rinpol	824.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	816.60		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	820.10		NIST Webbook
rinpol	814.00		NIST Webbook
tb	406.15 ± 0.40	K	NIST Webbook
tb	406.16 ± 0.10	K	NIST Webbook
tb	406.15 ± 0.50	K	NIST Webbook
tb	406.15 ± 1.50	K	NIST Webbook
tb	406.16 ± 0.03	K	NIST Webbook
tb	406.15 ± 1.00	K	NIST Webbook
tb	406.18	K	KDB
tb	406.20	K	NIST Webbook
tc	592.60	K	KDB
tc	592.60 ± 0.50	K	NIST Webbook
tc	592.65 ± 0.12	K	NIST Webbook
tf	152.06 ± 0.10	K	NIST Webbook
tf	152.06 ± 0.08	K	NIST Webbook
tf	150.95 ± 0.20	K	NIST Webbook
tf	152.06	K	KDB
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.13	J/mol×K	461.76	Joback Method
cpg	361.94	J/mol×K	582.85	Joback Method
cpg	349.03	J/mol×K	552.58	Joback Method
cpg	335.44	J/mol×K	522.31	Joback Method
cpg	321.15	J/mol×K	492.03	Joback Method
cpg	273.79	J/mol×K	401.21	Joback Method
cpg	290.35	J/mol×K	431.48	Joback Method
dvisc	0.0088523	Pa×s	203.21	Joback Method
dvisc	0.0027119	Pa×s	242.81	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	0.0512340	Pa×s	163.61	Joback Method
dvisc	0.0002468	Pa×s	401.21	Joback Method
hvapt	38.40	kJ/mol	369.00	NIST Webbook
hvapt	34.27	kJ/mol	406.20	KDB
rfi	1.41246		298.15	KDB
rhol	739.00	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	1.41481e+01
Coeff. B	-3.45501e+03
Coeff. C	-4.36320e+01
Temperature range (K), min.	292.90
Temperature range (K), max.	434.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	9.14194e+01
Coeff. B	-7.88184e+03
Coeff. C	-1.14363e+01
Coeff. D	7.87343e-06
Temperature range (K), min.	152.06
Temperature range (K), max.	592.15

Sources

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/research/kdb/hcprop/showprop.php?cmpid=95
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1186534&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=95

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