Hexane, 2,2,5,5-tetramethyl-

Other names:	2,2,5,5-Tetramethylhexane
	BINEOPENTYL
Inchi:	InChI=1S/C10H22/c1-9(2,3)7-8-10(4,5)6/h7-8H2,1-6H3
InchiKey:	HXQDUXXBVMMIKL-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CC(C)(C)CCC(C)(C)C
Mol. weight [g/mol]:	142.28
CAS:	1071-81-4

Physical Properties

Property code	Value	Unit	Source
af	0.3750		KDB
ap	356.150	K	KDB
gf	39.00	kJ/mol	Joback Method
hcg	6749.80	kJ/mol	KDB
hcn	6265.708	kJ/mol	KDB
hf	-285.00	kJ/mol	NIST Webbook
hfus	6.83	kJ/mol	Joback Method
hvap	43.50	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2190.00	kPa	KDB
pc	2190.00 ± 40.00	kPa	NIST Webbook
pc	2186.00 ± 10.00	kPa	NIST Webbook
rinpol	820.20		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	870.00		NIST Webbook
tb	410.70	K	NIST Webbook
tb	410.63	K	KDB
tb	410.60 ± 0.05	K	NIST Webbook

tb	409.65 ± 1.50	K	NIST Webbook
tc	581.45 ± 0.10	K	NIST Webbook
tc	581.40	K	KDB
tc	581.40 ± 0.50	K	NIST Webbook
tf	260.50	K	KDB
vc	0.574	m3/kmol	KDB
zc	0.2598160		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.63	J/mol×K	544.19	Joback Method
cpg	413.92	J/mol×K	605.42	Joback Method
cpg	400.18	J/mol×K	574.81	Joback Method
cpg	318.50	J/mol×K	421.74	Joback Method
cpg	336.71	J/mol×K	452.35	Joback Method
cpg	353.94	J/mol×K	482.97	Joback Method
cpg	370.23	J/mol×K	513.58	Joback Method
dvisc	0.0002658	Pa×s	421.74	Joback Method
dvisc	0.0006149	Pa×s	350.26	Joback Method
dvisc	0.0003889	Pa×s	386.00	Joback Method
dvisc	0.0186536	Pa×s	207.30	Joback Method
dvisc	0.0054554	Pa×s	243.04	Joback Method
dvisc	0.0021867	Pa×s	278.78	Joback Method
dvisc	0.0010789	Pa×s	314.52	Joback Method
hvapt	35.27	kJ/mol	410.60	KDB
rfi	1.40316		298.15	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39708e+01
Coeff. B	-3.24272e+03
Coeff. C	-6.38860e+01
Temperature range (K), min.	300.87

Temperature range (K), max.	438.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.62464e+01
Coeff. B	-8.41611e+03
Coeff. C	-1.20246e+01
Coeff. D	7.28060e-06
Temperature range (K), min.	300.00
Temperature range (K), max.	581.40

Sources

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=159
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/mol159.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1071814&Units=SI

Legend

af:	Acentric Factor
ap:	Aniline Point
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
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility