Hexane, 2,2,3,3-tetramethyl-

Other names: 2,2,3,3-Tetramethylhexane
Inchi: InChI=1S/C10H22/c1-7-8-10(5,6)9(2,3)4/h7-8H2,1-6H3
InchiKey: RMQHJMMCLSJULX-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCC(C)(C)C(C)(C)C
Mol. weight [g/mol]: 142.28
CAS: 13475-81-5

Physical Properties

Property code	Value	Unit	Source
af	0.3640		KDB
gf	39.00	kJ/mol	Joback Method
hcg	6776.66	kJ/mol	KDB
hcn	6292.569	kJ/mol	KDB
hf	-267.23	kJ/mol	Joback Method
hfus	6.83	kJ/mol	Joback Method
hvap	45.20	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2510.00 ± 40.00	kPa	NIST Webbook
pc	2510.00	kPa	KDB
pc	2510.00 ± 40.00	kPa	NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	928.80		NIST Webbook
rinpol	929.00		NIST Webbook
tb	433.46 ± 0.10	K	NIST Webbook
tb	433.00 ± 0.60	K	NIST Webbook
tb	433.48	K	KDB
tb	431.20 ± 1.50	K	NIST Webbook
tc	623.00	K	KDB
tc	623.00 ± 0.50	K	NIST Webbook
tc	623.05 ± 0.40	K	NIST Webbook
tf	219.12 ± 0.10	K	NIST Webbook
tf	219.15 ± 0.03	K	NIST Webbook

tf	219.00	K	KDB
tf	219.15 ± 0.05	K	NIST Webbook
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.92	J/mol×K	605.42	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
cpg	385.63	J/mol×K	544.19	Joback Method
cpg	400.18	J/mol×K	574.81	Joback Method
dvisc	0.0002658	Pa×s	421.74	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
dvisc	0.0006149	Pa×s	350.26	Joback Method
dvisc	0.0003889	Pa×s	386.00	Joback Method
hvapt	36.36	kJ/mol	433.50	KDB
rfi	1.42600		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	1.42388e+01
Coeff. B	-3.64182e+03
Coeff. C	-5.49330e+01
Temperature range (K), min.	315.97
Temperature range (K), max.	462.87

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.13601e+01
Coeff. B	-8.39949e+03
Coeff. C	-1.13148e+01
Coeff. D	7.11760e-06
Temperature range (K), min.	314.00
Temperature range (K), max.	623.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13475815&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=154
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/mol154.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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