Hexane, 2,2,4-trimethyl-

Other names: 2,2,4-Trimethylhexane
Inchi: InChI=1S/C9H20/c1-6-8(2)7-9(3,4)5/h8H,6-7H2,1-5H3
InchiKey: AFTPEBDOGXRMNQ-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCC(C)CC(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 16747-26-5

Physical Properties

Property code	Value	Unit	Source
af	0.3210		KDB
ap	351.150	K	KDB
chl	-6117.05 ± 0.84	kJ/mol	NIST Webbook
gf	22.52	kJ/mol	KDB
hcg	6117.05	kJ/mol	KDB
hcn	5676.935	kJ/mol	KDB
hf	-243.40	kJ/mol	KDB
hfl	-282.80 ± 1.00	kJ/mol	NIST Webbook
hfus	8.13	kJ/mol	Joback Method
hvap	40.70	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2380.00	kPa	KDB
rinpol	789.20		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	794.20		NIST Webbook
rinpol	794.30		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	790.70		NIST Webbook
rinpol	788.80		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	789.00		NIST Webbook

rinpol	792.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	786.50		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	790.80		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	792.80		NIST Webbook
rinpol	791.60		NIST Webbook
rinpol	789.61		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	792.80		NIST Webbook
rinpol	792.80		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
tb	399.70	K	KDB

tc	573.70	K	KDB
tf	149.75 ± 0.20	K	NIST Webbook
tf	149.77 ± 1.50	K	NIST Webbook
tf	153.00	K	KDB
tf	153.15 ± 0.40	K	NIST Webbook
tf	143.62 ± 0.60	K	NIST Webbook
vc	0.507	m3/kmol	KDB
zc	0.2527670		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.89	J/mol×K	401.65	Joback Method
cpg	289.98	J/mol×K	431.23	Joback Method
cpg	305.33	J/mol×K	460.81	Joback Method
cpg	319.96	J/mol×K	490.39	Joback Method
cpg	333.90	J/mol×K	519.97	Joback Method
cpg	347.18	J/mol×K	549.55	Joback Method
cpg	359.82	J/mol×K	579.13	Joback Method
hvapt	34.02	kJ/mol	399.70	KDB
hvapt	39.50	kJ/mol	349.00	NIST Webbook
hvapt	41.00	kJ/mol	315.50	NIST Webbook
hvapt	40.50	kJ/mol	270.50	NIST Webbook
rfi	1.40100		298.15	KDB
rhol	720.00	kg/m3	289.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41733e+01
Coeff. B	-3.36653e+03
Coeff. C	-4.73560e+01
Temperature range (K), min.	289.80
Temperature range (K), max.	427.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.11430e+01
Coeff. B	-7.88090e+03
Coeff. C	-1.13543e+01
Coeff. D	7.59218e-06
Temperature range (K), min.	291.00
Temperature range (K), max.	573.50

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=83
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=83
The pressure dependence of viscosity for 2,2,4 trimethylhexane to 1 GPa along the 20°C isotherm:	https://www.doi.org/10.1016/j.fluid.2019.01.021
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747265&Units=SI

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hfl:	Liquid phase 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
zc:	Critical Compressibility