Hexane, 3,3,4-trimethyl-

Other names: 3,3,4-Trimethylhexane
Inchi: InChI=1S/C9H20/c1-6-8(3)9(4,5)7-2/h8H,6-7H2,1-5H3
InchiKey: ARWOOWBJJKVYOV-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCC(C)C(C)(C)CC
Mol. weight [g/mol]: 128.26
CAS: 16747-31-2

Physical Properties

Property code	Value	Unit	Source
chl	-6122.36 ± 0.75	kJ/mol	NIST Webbook
gf	25.30	kJ/mol	Joback Method
hf	-243.12	kJ/mol	Joback Method
hfl	-277.50 ± 0.92	kJ/mol	NIST Webbook
hfus	8.13	kJ/mol	Joback Method
hvap	42.20	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	851.70		NIST Webbook
rinpol	857.10		NIST Webbook
rinpol	850.80		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	855.10		NIST Webbook
rinpol	854.40		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	855.00		NIST Webbook

rinpol	858.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	848.00		NIST Webbook
ripol	816.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	816.00		NIST Webbook
tb	413.05 ± 0.50	K	NIST Webbook
tb	413.57 ± 0.15	K	NIST Webbook
tc	579.13	K	Joback Method
tf	171.95 ± 0.05	K	NIST Webbook
vc	0.522	m3/kmol	Joback Method

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
dvisc	0.0222427	Pa×s	178.61	Joback Method
dvisc	0.0055664	Pa×s	215.78	Joback Method
dvisc	0.0020930	Pa×s	252.96	Joback Method
dvisc	0.0010112	Pa×s	290.13	Joback Method
dvisc	0.0005763	Pa×s	327.30	Joback Method
dvisc	0.0003684	Pa×s	364.48	Joback Method
dvisc	0.0002558	Pa×s	401.65	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38943e+01
Coeff. B	-3.23887e+03
Coeff. C	-6.44510e+01
Temperature range (K), min.	302.49
Temperature range (K), max.	441.82

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.53062e+01
Coeff. B	-7.82480e+03
Coeff. C	-1.04380e+01
Coeff. D	6.54368e-06
Temperature range (K), min.	300.15
Temperature range (K), max.	602.30

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=89

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747312&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=89

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume