Hexane, 2,3,3-trimethyl-

Other names:	2,3,3-Trimethylheptane
	2,3,3-Trimethylhexane
Inchi:	InChI=1S/C9H20/c1-6-7-9(4,5)8(2)3/h8H,6-7H2,1-5H3
InchiKey:	DJYSEQMMCZAKGT-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCCC(C)(C)C(C)C
Mol. weight [g/mol]:	128.26
CAS:	16747-28-7

Physical Properties

Property code	Value	Unit	Source
chl	-6118.81 ± 0.84	kJ/mol	NIST Webbook
gf	25.30	kJ/mol	Joback Method
hf	-243.12	kJ/mol	Joback Method
hfl	-281.10 ± 1.00	kJ/mol	NIST Webbook
hfus	8.13	kJ/mol	Joback Method
hvap	42.10	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	842.00		NIST Webbook
rinpol	841.70		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.90		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	840.00		NIST Webbook

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rinpol	840.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	843.60		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	839.10		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	839.70		NIST Webbook
rinpol	840.70		NIST Webbook
tb	409.95 ± 0.40	K	NIST Webbook
tb	409.45 ± 0.50	K	NIST Webbook
tb	410.90	K	NIST Webbook
tb	410.75 ± 1.00	K	NIST Webbook
tc	579.13	K	Joback Method
tf	156.35 ± 0.05	K	NIST Webbook
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.18	J/mol×K	549.55	Joback Method
cpg	359.82	J/mol×K	579.13	Joback Method
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
dvisc	0.0002558	Pa×s	401.65	Joback Method
dvisc	0.0003684	Pa×s	364.48	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
hvapt	39.40	kJ/mol	355.00	NIST Webbook
hvapt	44.20	kJ/mol	270.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40436e+01
Coeff. B	-3.35266e+03
Coeff. C	-5.51290e+01
Temperature range (K), min.	298.85
Temperature range (K), max.	439.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.11918e+01
Coeff. B	-7.47165e+03
Coeff. C	-9.89411e+00
Coeff. D	6.84567e-06
Temperature range (K), min.	238.15
Temperature range (K), max.	596.00

Sources

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/mol85.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16747287&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=85

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume