

Hexane, 2,3,4-trimethyl-

Other names:	2,3,4-Trimethylhexane
Inchi:	InChI=1S/C9H20/c1-6-8(4)9(5)7(2)3/h7-9H,6H2,1-5H3
InchiKey:	RUTNOQHQISEBGT-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCC(C)C(C)C(C)C
Mol. weight [g/mol]:	128.26
CAS:	921-47-1

Physical Properties

Property code	Value	Unit	Source
gf	17.58	kJ/mol	Joback Method
hf	-244.93	kJ/mol	Joback Method
hfus	8.50	kJ/mol	Joback Method
hvap	42.70	kJ/mol	NIST Webbook
log10ws	-2.86		Crippen Method
logp	3.325		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	850.05		NIST Webbook
rinpol	851.40		NIST Webbook
rinpol	848.30		NIST Webbook
rinpol	848.40		NIST Webbook
rinpol	849.90		NIST Webbook
rinpol	850.10		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	849.70		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	843.00		NIST Webbook

rinpol	847.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	849.30		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	850.20		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.20		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	851.40		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	845.80		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	848.00		NIST Webbook
tb	412.21 ± 0.30	K	NIST Webbook
tb	412.00 ± 1.50	K	NIST Webbook
tb	410.85 ± 0.70	K	NIST Webbook
tb	410.35 ± 0.40	K	NIST Webbook
tb	412.25 ± 0.30	K	NIST Webbook
tb	412.21 ± 0.60	K	NIST Webbook
tc	578.35	K	Joback Method
tf	146.19	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.44	J/mol×K	404.00	Joback Method
cpg	287.79	J/mol×K	433.06	Joback Method

cpg	302.55	J/mol×K	462.12	Joback Method
cpg	316.72	J/mol×K	491.17	Joback Method
cpg	330.33	J/mol×K	520.23	Joback Method
cpg	343.38	J/mol×K	549.29	Joback Method
cpg	355.89	J/mol×K	578.35	Joback Method
dvisc	0.0558851	Pa×s	146.19	Joback Method
dvisc	0.0077512	Pa×s	189.16	Joback Method
dvisc	0.0022339	Pa×s	232.13	Joback Method
dvisc	0.0009496	Pa×s	275.10	Joback Method
dvisc	0.0005086	Pa×s	318.06	Joback Method
dvisc	0.0003161	Pa×s	361.03	Joback Method
dvisc	0.0002173	Pa×s	404.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41855e+01
Coeff. B	-3.44620e+03
Coeff. C	-5.19900e+01
Temperature range (K), min.	299.95
Temperature range (K), max.	440.34

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.02224e+01
Coeff. B	-8.04411e+03
Coeff. C	-1.11797e+01
Coeff. D	7.24323e-06
Temperature range (K), min.	300.15
Temperature range (K), max.	594.50

Sources

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

KDB:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=86
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C921471&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.therc.org/research/kdb/hcprop/showprop.php?cmpid=86
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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