Heptane, 3,3-dimethyl-

Other names: 3,3-Dimethylheptane
Inchi: InChI=1S/C9H20/c1-5-7-8-9(3,4)6-2/h5-8H2,1-4H3
InchiKey: BVAKDOXCVSMKHE-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCCC(C)(C)CC
Mol. weight [g/mol]: 128.26
CAS: 4032-86-4

Physical Properties

Property code	Value	Unit	Source
af	0.3790		KDB
ap	347.150	K	KDB
gf	27.74	kJ/mol	Joback Method
hcg	6116.21	kJ/mol	KDB
hcn	5676.098	kJ/mol	KDB
hf	-237.84	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	42.60	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2430.00	kPa	KDB
rinpol	839.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	836.50		NIST Webbook
rinpol	839.10		NIST Webbook
rinpol	839.10		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	837.30		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	836.50		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook

rinpol	832.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	844.60		NIST Webbook
rinpol	839.70		NIST Webbook
rinpol	834.60		NIST Webbook
rinpol	836.13		NIST Webbook
rinpol	836.23		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	835.60		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	839.70		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	839.10		NIST Webbook
rinpol	835.60		NIST Webbook
tb	410.20	K	KDB
tc	588.40	K	KDB

tf	170.00	K	KDB
vc	0.506	m3/kmol	KDB
zc	0.2513320		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.39	J/mol×K	546.65	Joback Method
cpg	357.75	J/mol×K	575.56	Joback Method
cpg	273.99	J/mol×K	402.09	Joback Method
cpg	289.63	J/mol×K	431.00	Joback Method
cpg	304.56	J/mol×K	459.91	Joback Method
cpg	318.82	J/mol×K	488.82	Joback Method
cpg	332.42	J/mol×K	517.74	Joback Method
dvisc	0.0002652	Pa×s	402.09	Joback Method
dvisc	0.0003685	Pa×s	367.34	Joback Method
dvisc	0.0112198	Pa×s	193.61	Joback Method
dvisc	0.0037384	Pa×s	228.36	Joback Method
dvisc	0.0016651	Pa×s	263.10	Joback Method
dvisc	0.0008957	Pa×s	297.85	Joback Method
dvisc	0.0005485	Pa×s	332.60	Joback Method
hvapt	35.31	kJ/mol	410.20	KDB
rfi	1.40630		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49951e+01
Coeff. B	-3.68576e+03
Coeff. C	-5.52550e+01
Temperature range (K), min.	305.86
Temperature range (K), max.	435.87

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.96890e+01
Coeff. B	-8.03316e+03
Coeff. C	-1.10809e+01
Coeff. D	7.03669e-06
Temperature range (K), min.	319.00
Temperature range (K), max.	458.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4032864&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=74
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/mol74.mol

Legend

af:	Acentric Factor
ap:	Aniline Point
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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure

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

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