Heptane, 2,2-dimethyl-

Other names: 2,2-Dimethylheptane
Inchi: InChI=1S/C9H20/c1-5-6-7-8-9(2,3)4/h5-8H2,1-4H3
InchiKey: PSABUFWDVWCFDP-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCCCC(C)(C)C
Mol. weight [g/mol]: 128.26
CAS: 1071-26-7

Physical Properties

Property code	Value	Unit	Source
af	0.3900		KDB
ap	352.150	K	KDB
chl	-6111.74 ± 0.84	kJ/mol	NIST Webbook
gf	16.75	kJ/mol	KDB
hcg	6111.74	kJ/mol	KDB
hcn	5671.622	kJ/mol	KDB
hf	-247.00	kJ/mol	KDB
hf	-246.10	kJ/mol	NIST Webbook
hfl	-288.20 ± 1.00	kJ/mol	NIST Webbook
hfus	11.65	kJ/mol	Joback Method
hvap	42.30	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2350.00 ± 41.37	kPa	NIST Webbook
pc	2350.00	kPa	KDB
pc	2350.00 ± 40.00	kPa	NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	815.10		NIST Webbook
rinpol	816.10		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	817.10		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	816.50		NIST Webbook

rinpol	817.10	NIST Webbook
rinpol	817.70	NIST Webbook
rinpol	811.60	NIST Webbook
rinpol	814.20	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	810.00	NIST Webbook
rinpol	811.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	813.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	808.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	812.00	NIST Webbook
rinpol	829.90	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	824.70	NIST Webbook
rinpol	818.90	NIST Webbook
rinpol	816.53	NIST Webbook
rinpol	818.34	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	815.00	NIST Webbook
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rinpol	818.00	NIST Webbook
rinpol	818.00	NIST Webbook
rinpol	815.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	819.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	817.00	NIST Webbook

rinpol	816.00		NIST Webbook
rinpol	820.00		NIST Webbook
tb	405.80	K	KDB
tc	576.69 ± 0.50	K	NIST Webbook
tc	576.70 ± 0.50	K	NIST Webbook
tc	576.70	K	KDB
tf	160.00	K	KDB
vc	0.528	m3/kmol	KDB
zc	0.2590160		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.42	J/mol×K	517.74	Joback Method
cpg	357.75	J/mol×K	575.56	Joback Method
cpg	345.39	J/mol×K	546.65	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
dvisc	0.0005485	Pa×s	332.60	Joback Method
dvisc	0.0003685	Pa×s	367.34	Joback Method
dvisc	0.0002652	Pa×s	402.09	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
hvapt	34.77	kJ/mol	405.90	KDB
rfi	1.39930		298.15	KDB
rhol	711.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43315e+01

Coeff. B	-3.46987e+03
Coeff. C	-4.86060e+01
Temperature range (K), min.	295.68
Temperature range (K), max.	433.29

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02542e+02
Coeff. B	-8.54380e+03
Coeff. C	-1.30419e+01
Coeff. D	8.85387e-06
Temperature range (K), min.	160.15
Temperature range (K), max.	576.80

Sources

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=69
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/mol69.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1071267&Units=SI

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
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

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