Heptane, 3,5-dimethyl-

Other names: 3,5-Dimethylheptane
Inchi: InChI=1S/C9H20/c1-5-8(3)7-9(4)6-2/h8-9H,5-7H2,1-4H3
InchiKey: DZJTZGHZAWTWGA-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCC(C)CC(C)CC
Mol. weight [g/mol]: 128.26
CAS: 926-82-9

Physical Properties

Property code	Value	Unit	Source
af	0.3850		KDB
gf	20.02	kJ/mol	Joback Method
hcg	6118.31	kJ/mol	KDB
hcn	5678.190	kJ/mol	KDB
hf	-239.65	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	43.30	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2400.00	kPa	KDB
rinpol	834.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	833.70		NIST Webbook
rinpol	834.60		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.60		NIST Webbook
rinpol	845.60		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	834.00		NIST Webbook

rinpol	840.20		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	837.20		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	834.40		NIST Webbook
rinpol	838.10		NIST Webbook
rinpol	837.30		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	837.40		NIST Webbook
rinpol	837.60		NIST Webbook
rinpol	838.10		NIST Webbook
tb	408.05 ± 1.00	K	NIST Webbook
tb	408.65 ± 1.00	K	NIST Webbook
tb	409.20	K	NIST Webbook
tb	409.20	K	KDB
tb	409.15 ± 0.50	K	NIST Webbook
tc	583.20	K	KDB
tf	170.00	K	KDB
vc	0.510	m3/kmol	KDB
zc	0.2524220		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.86	J/mol×K	574.89	Joback Method
cpg	287.44	J/mol×K	432.85	Joback Method
cpg	301.80	J/mol×K	461.26	Joback Method
cpg	315.61	J/mol×K	489.67	Joback Method
cpg	328.88	J/mol×K	518.07	Joback Method
cpg	341.62	J/mol×K	546.48	Joback Method
cpg	272.52	J/mol×K	404.44	Joback Method

dvisc	0.0003168	Pa×s	363.90	Joback Method
dvisc	0.0004846	Pa×s	323.36	Joback Method
dvisc	0.0008373	Pa×s	282.81	Joback Method
dvisc	0.0017372	Pa×s	242.27	Joback Method
dvisc	0.0048330	Pa×s	201.73	Joback Method
dvisc	0.0002255	Pa×s	404.44	Joback Method
dvisc	0.0224972	Pa×s	161.19	Joback Method
hvapt	35.65	kJ/mol	409.20	KDB
rfi	1.40440		298.15	KDB
rhol	694.50	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	669.70	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	661.20	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	734.00	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	726.20	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	718.40	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	710.50	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	702.50	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	710.50	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	718.40	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	726.30	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	734.10	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	678.00	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	702.50	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	686.30	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41770e+01
Coeff. B	-3.36017e+03
Coeff. C	-5.76290e+01
Temperature range (K), min.	299.55
Temperature range (K), max.	436.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.65761e+01
Coeff. B	-8.38639e+03
Coeff. C	-1.20980e+01
Coeff. D	7.74710e-06
Temperature range (K), min.	299.15
Temperature range (K), max.	583.20

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=76
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=76
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926829&Units=SI
Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:	https://www.doi.org/10.1021/je400274f

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility