Heptane, 3,4-dimethyl-

Other names: 3,4-Dimethylheptane
Inchi: InChI=1S/C9H20/c1-5-7-9(4)8(3)6-2/h8-9H,5-7H2,1-4H3
InchiKey: MAKRYGRRIKSDES-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCC(C)C(C)CC
Mol. weight [g/mol]: 128.26
CAS: 922-28-1

Physical Properties

Property code	Value	Unit	Source
af	0.3790		KDB
ap	343.150	K	KDB
gf	20.02	kJ/mol	Joback Method
hcg	6121.95	kJ/mol	KDB
hcn	5681.830	kJ/mol	KDB
hf	-239.65	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	43.60	kJ/mol	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2460.00	kPa	KDB
rinpol	859.20		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	859.40		NIST Webbook
rinpol	859.90		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	858.50		NIST Webbook
rinpol	858.50		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	858.00		NIST Webbook
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rinpol	860.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	868.40		NIST Webbook
rinpol	869.20		NIST Webbook
rinpol	858.80		NIST Webbook
rinpol	856.80		NIST Webbook
rinpol	857.61		NIST Webbook
rinpol	857.79		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	858.80		NIST Webbook
rinpol	860.00		NIST Webbook
tb	413.80	K	KDB
tb	413.25 ± 0.50	K	NIST Webbook
tb	413.85 ± 0.30	K	NIST Webbook
tb	413.80	K	NIST Webbook
tc	591.90	K	KDB
tf	170.00	K	KDB
vc	0.503	m3/kmol	KDB
zc	0.2514310		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.86	J/mol×K	574.89	Joback Method
cpg	272.52	J/mol×K	404.44	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
dvisc	0.0002255	Pa×s	404.44	Joback Method
dvisc	0.0224972	Pa×s	161.19	Joback Method
dvisc	0.0048330	Pa×s	201.73	Joback Method
dvisc	0.0017372	Pa×s	242.27	Joback Method
dvisc	0.0008373	Pa×s	282.81	Joback Method
dvisc	0.0004846	Pa×s	323.36	Joback Method
dvisc	0.0003168	Pa×s	363.90	Joback Method
hvapt	36.36	kJ/mol	413.80	KDB
rfi	1.40890		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42531e+01
Coeff. B	-3.46685e+03
Coeff. C	-5.39320e+01
Temperature range (K), min.	302.18
Temperature range (K), max.	441.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.56536e+01
Coeff. B	-8.37141e+03
Coeff. C	-1.19715e+01
Coeff. D	7.76203e-06
Temperature range (K), min.	302.15
Temperature range (K), max.	591.90

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=75
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C922281&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=75
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

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
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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