

Heptane, 2,3-dimethyl-

Other names:	2,3-Dimethylheptane
Inchi:	InChI=1S/C9H20/c1-5-6-7-9(4)8(2)3/h8-9H,5-7H2,1-4H3
InchiKey:	WBRFDUJXCLCKPX-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCCCC(C)C(C)C
Mol. weight [g/mol]:	128.26
CAS:	3074-71-3

Physical Properties

Property code	Value	Unit	Source
af	0.3850		KDB
ap	346.350	K	KDB
gf	20.02	kJ/mol	Joback Method
hcg	6119.77	kJ/mol	KDB
hcn	5679.655	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	2400.00	kPa	KDB
rinpola	835.10		NIST Webbook
rinpola	857.20		NIST Webbook
rinpola	854.00		NIST Webbook
rinpola	855.50		NIST Webbook
rinpola	855.30		NIST Webbook
rinpola	855.30		NIST Webbook
rinpola	854.80		NIST Webbook
rinpola	851.00		NIST Webbook
rinpola	852.00		NIST Webbook
rinpola	852.00		NIST Webbook
rinpola	853.00		NIST Webbook
rinpola	854.00		NIST Webbook
rinpola	858.00		NIST Webbook
rinpola	856.00		NIST Webbook
rinpola	856.00		NIST Webbook

rinpol	857.00	NIST Webbook
rinpol	849.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	857.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	867.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	846.50	NIST Webbook
rinpol	853.10	NIST Webbook
rinpol	854.90	NIST Webbook
rinpol	857.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	853.50	NIST Webbook
rinpol	857.30	NIST Webbook
rinpol	856.89	NIST Webbook
rinpol	857.42	NIST Webbook
rinpol	855.86	NIST Webbook
rinpol	856.70	NIST Webbook
rinpol	857.24	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	855.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	864.00	NIST Webbook
rinpol	859.00	NIST Webbook
rinpol	853.00	NIST Webbook
rinpol	855.20	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	862.00	NIST Webbook
rinpol	860.00	NIST Webbook
rinpol	858.00	NIST Webbook
rinpol	854.00	NIST Webbook
rinpol	856.00	NIST Webbook
rinpol	853.00	NIST Webbook

rinpol	837.20		NIST Webbook
rinpol	856.05		NIST Webbook
tb	413.70 ± 0.30	K	NIST Webbook
tb	413.15 ± 1.00	K	NIST Webbook
tb	413.85 ± 0.30	K	NIST Webbook
tb	413.80 ± 0.30	K	NIST Webbook
tb	411.45 ± 1.50	K	NIST Webbook
tb	413.15 ± 1.00	K	NIST Webbook
tb	413.70	K	KDB
tb	413.30 ± 0.70	K	NIST Webbook
tc	589.60	K	KDB
tf	160.00	K	KDB
vc	0.515	m ³ /kmol	KDB
zc	0.2521300		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	353.86	J/mol×K	574.89	Joback Method
dvisc	0.0048330	Paxs	201.73	Joback Method
dvisc	0.0224972	Paxs	161.19	Joback Method
dvisc	0.0017372	Paxs	242.27	Joback Method
dvisc	0.0008373	Paxs	282.81	Joback Method
dvisc	0.0004846	Paxs	323.36	Joback Method
dvisc	0.0003168	Paxs	363.90	Joback Method
dvisc	0.0002255	Paxs	404.44	Joback Method
hvapt	36.11	kJ/mol	413.70	KDB
rfi	1.40620		298.15	KDB

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41411e+01
Coeff. B	-3.36520e+03
Coeff. C	-6.02750e+01
Temperature range (K), min.	303.19
Temperature range (K), max.	441.40

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.79990e+01
Coeff. B	-8.48564e+03
Coeff. C	-1.23212e+01
Coeff. D	8.00191e-06
Temperature range (K), min.	302.15
Temperature range (K), max.	589.60

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=70
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3074713&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=70
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws

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
mcpvol:	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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