Hexane, 3-ethyl-

Other names: 3-Ethylhexane
Inchi: InChI=1S/C8H18/c1-4-7-8(5-2)6-3/h8H,4-7H2,1-3H3
InchiKey: SFRKSDZMZHIISH-UHFFFAOYSA-N
Formula: C8H18
SMILES: CCCC(CC)CC
Mol. weight [g/mol]: 114.23
CAS: 619-99-8

Physical Properties

Property code	Value	Unit	Source
af	0.3610		KDB
ap	341.850	K	KDB
chl	-5432.10	kJ/mol	NIST Webbook
chl	-5470.12 ± 0.96	kJ/mol	NIST Webbook
chl	-5262.00	kJ/mol	NIST Webbook
gf	16.94	kJ/mol	KDB
hcg	5470.12	kJ/mol	KDB
hcn	5073.979	kJ/mol	KDB
hf	-211.00	kJ/mol	KDB
hf	-210.90 ± 1.20	kJ/mol	NIST Webbook
hfl	-250.50 ± 1.10	kJ/mol	NIST Webbook
hfus	12.95	kJ/mol	Joback Method
hvap	39.69	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
hvap	33.00	kJ/mol	NIST Webbook
hvap	39.69	kJ/mol	NIST Webbook
hvap	39.60 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2610.00 ± 40.00	kPa	NIST Webbook
pc	2610.00	kPa	KDB
pc	2607.90 ± 40.53	kPa	NIST Webbook
rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rhoc	251.30 ± 4.57	kg/m3	NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	775.00		NIST Webbook

rinpol	773.00	NIST Webbook
rinpol	775.30	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.20	NIST Webbook
rinpol	773.40	NIST Webbook
rinpol	775.70	NIST Webbook
rinpol	775.70	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.80	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	775.30	NIST Webbook
rinpol	775.30	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	776.90	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.20	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	772.00	NIST Webbook
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rinpol	774.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	773.40		NIST Webbook
rinpol	772.90		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	769.70		NIST Webbook
rinpol	770.10		NIST Webbook
rinpol	771.44		NIST Webbook
rinpol	773.69		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	774.01		NIST Webbook
rinpol	774.57		NIST Webbook
rinpol	774.94		NIST Webbook
rinpol	773.78		NIST Webbook
rinpol	774.37		NIST Webbook
rinpol	774.75		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	770.00		NIST Webbook
tb	391.70	K	KDB
tb	391.85 ± 0.30	K	NIST Webbook
tb	391.85 ± 0.20	K	NIST Webbook
tb	391.68 ± 0.10	K	NIST Webbook
tb	391.68 ± 0.02	K	NIST Webbook
tb	391.90 ± 0.00	K	NIST Webbook

tb	391.70 ± 0.15	K	NIST Webbook
tb	391.65 ± 0.50	K	NIST Webbook
tb	391.85 ± 0.50	K	NIST Webbook
tb	391.80 ± 0.40	K	NIST Webbook
tb	391.69 ± 0.20	K	NIST Webbook
tb	391.97 ± 0.20	K	NIST Webbook
tb	391.68 ± 0.20	K	NIST Webbook
tb	391.70	K	NIST Webbook
tb	391.70	K	NIST Webbook
tb	391.55 ± 0.20	K	NIST Webbook
tc	565.42 ± 0.40	K	NIST Webbook
tc	565.40	K	NIST Webbook
tc	565.50 ± 0.50	K	NIST Webbook
tc	565.50	K	KDB
tf	164.92	K	Joback Method
vc	0.455	m3/kmol	NIST Webbook
vc	0.455	m3/kmol	KDB
zc	0.2525710		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.42	J/mol×K	397.10	NIST Webbook
cpg	269.87	J/mol×K	462.70	NIST Webbook
cpg	298.74	J/mol×K	522.70	NIST Webbook
dvisc	0.0002373	Pa×s	382.00	Joback Method
dvisc	0.0105616	Pa×s	164.92	Joback Method
dvisc	0.0031758	Pa×s	201.10	Joback Method
dvisc	0.0013776	Pa×s	237.28	Joback Method
dvisc	0.0007454	Pa×s	273.46	Joback Method
dvisc	0.0004656	Pa×s	309.64	Joback Method
dvisc	0.0003209	Pa×s	345.82	Joback Method
hvapt	42.40	kJ/mol	321.00	NIST Webbook
hvapt	33.61	kJ/mol	391.70	KDB
hvapt	33.59	kJ/mol	391.70	NIST Webbook
hvapt	38.20	kJ/mol	353.50	NIST Webbook
rfi	1.39919		298.15	KDB
rhol	718.00	kg/m3	289.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42298e+01
Coeff. B	-3.26994e+03
Coeff. C	-5.14790e+01
Temperature range (K), min.	286.01
Temperature range (K), max.	418.13

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.99778e+01
Coeff. B	-7.73243e+03
Coeff. C	-1.11883e+01
Coeff. D	7.70935e-06
Temperature range (K), min.	250.00
Temperature range (K), max.	565.40

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol50.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619998&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=50

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rhoc:	Critical density
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