Heptane, 3-ethyl-

Other names: 3-Ethylheptane
Inchi: InChI=1S/C9H20/c1-4-7-8-9(5-2)6-3/h9H,4-8H2,1-3H3
InchiKey: PSVQKOKKLWHNRP-UHFFFAOYSA-N
Formula: C9H20
SMILES: CCCCC(CC)CC
Mol. weight [g/mol]: 128.26
CAS: 15869-80-4

Physical Properties

Property code	Value	Unit	Source
af	0.4160		KDB
ap	346.150	K	KDB
gf	22.46	kJ/mol	Joback Method
hcg	6123.95	kJ/mol	KDB
hcn	5683.839	kJ/mol	KDB
hf	-234.37	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	44.50	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2330.00	kPa	KDB
rinpol	865.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	867.10		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	872.40		NIST Webbook

rinpol	870.30		NIST Webbook
rinpol	866.88		NIST Webbook
rinpol	869.57		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	871.30		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	870.50		NIST Webbook
rinpol	870.74		NIST Webbook
rinpol	867.40		NIST Webbook
rinpol	871.59		NIST Webbook
rinpol	870.44		NIST Webbook
rinpol	870.98		NIST Webbook
rinpol	871.37		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	867.40		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	871.10		NIST Webbook
rinpol	867.40		NIST Webbook
rinpol	866.60		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	871.27		NIST Webbook
rinpol	865.00		NIST Webbook
tb	416.20	K	KDB
tb	416.25 ± 0.20	K	NIST Webbook
tb	416.25 ± 0.40	K	NIST Webbook
tb	416.75 ± 0.30	K	NIST Webbook
tc	587.50	K	KDB
tf	160.00	K	KDB
vc	0.533	m3/kmol	KDB
zc	0.2544750		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.60	J/mol×K	404.88	Joback Method
cpg	287.11	J/mol×K	432.66	Joback Method
cpg	301.08	J/mol×K	460.44	Joback Method
cpg	314.53	J/mol×K	488.22	Joback Method
cpg	327.48	J/mol×K	516.01	Joback Method
cpg	339.92	J/mol×K	543.79	Joback Method
cpg	351.89	J/mol×K	571.57	Joback Method
dvisc	0.0032357	Pa×s	214.31	Joback Method
dvisc	0.0108182	Pa×s	176.19	Joback Method
dvisc	0.0013934	Pa×s	252.42	Joback Method
dvisc	0.0007485	Pa×s	290.53	Joback Method
dvisc	0.0004644	Pa×s	328.65	Joback Method
dvisc	0.0003182	Pa×s	366.76	Joback Method
dvisc	0.0002341	Pa×s	404.88	Joback Method
hvapt	36.74	kJ/mol	416.20	KDB
rfi	1.40700		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46094e+01
Coeff. B	-3.74920e+03
Coeff. C	-4.10930e+01
Temperature range (K), min.	302.88
Temperature range (K), max.	444.33

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.26259e+01
Coeff. B	-7.54929e+03
Coeff. C	-8.38301e+00

Coeff. D	4.01087e-06
Temperature range (K), min.	158.25
Temperature range (K), max.	590.00

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=67
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/mol67.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869804&Units=SI

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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