Hexane, 3-ethyl-3-methyl-

Other names:	3-Ethyl-3-methylhexane
	3-METHYL-3-ETHYLHEXANE
Inchi:	InChI=1S/C9H20/c1-5-8-9(4,6-2)7-3/h5-8H2,1-4H3
InchiKey:	CYWROHZCELEGSE-UHFFFAOYSA-N
Formula:	C9H20
SMILES:	CCCC(C)(CC)CC
Mol. weight [g/mol]:	128.26
CAS:	3074-76-8

Physical Properties

Property code	Value	Unit	Source
af	0.3520		KDB
gf	27.74	kJ/mol	Joback Method
hcg	6122.03	kJ/mol	KDB
hcn	5681.914	kJ/mol	KDB
hf	-237.84	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	42.90	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.613		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2550.00	kPa	KDB
rinpol	856.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	856.50		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	854.80		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	855.50		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	852.00		NIST Webbook

rinpol	851.00		NIST Webbook
rinpol	855.50		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	855.00		NIST Webbook
tb	413.80	K	KDB
tb	413.75 ± 0.50	K	NIST Webbook
tc	597.50	K	KDB
tf	160.00	K	KDB
vc	0.487	m3/kmol	KDB
zc	0.2499740		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.39	J/mol×K	546.65	Joback Method
cpg	332.42	J/mol×K	517.74	Joback Method
cpg	318.82	J/mol×K	488.82	Joback Method
cpg	304.56	J/mol×K	459.91	Joback Method
cpg	289.63	J/mol×K	431.00	Joback Method
cpg	273.99	J/mol×K	402.09	Joback Method
cpg	357.75	J/mol×K	575.56	Joback Method
dvisc	0.0112198	Pa×s	193.61	Joback Method
dvisc	0.0002652	Pa×s	402.09	Joback Method
dvisc	0.0003685	Pa×s	367.34	Joback Method
dvisc	0.0005485	Pa×s	332.60	Joback Method
dvisc	0.0008957	Pa×s	297.85	Joback Method
dvisc	0.0016651	Pa×s	263.10	Joback Method
dvisc	0.0037384	Pa×s	228.36	Joback Method
hvapt	35.73	kJ/mol	413.80	KDB
rfi	1.41200		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42025e+01
Coeff. B	-3.46967e+03

Coeff. C	-5.17400e+01
Temperature range (K), min.	301.09
Temperature range (K), max.	441.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.94498e+01
Coeff. B	-8.04520e+03
Coeff. C	-1.10523e+01
Coeff. D	7.04742e-06
Temperature range (K), min.	301.15
Temperature range (K), max.	597.50

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3074768&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=80
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/mol80.mol

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
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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