

Octane, 3-ethyl-

Other names:	3-Ethyloctane
Inchi:	InChI=1S/C10H22/c1-4-7-8-9-10(5-2)6-3/h10H,4-9H2,1-3H3
InchiKey:	OEYGTUAKNZFCDJ-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCC(CC)CC
Mol. weight [g/mol]:	142.28
CAS:	5881-17-4

Physical Properties

Property code	Value	Unit	Source
af	0.4460		KDB
ap	348.150	K	KDB
gf	30.88	kJ/mol	Joback Method
hcg	6773.98	kJ/mol	KDB
hcn	6289.850	kJ/mol	KDB
hf	-255.01	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	49.00	kJ/mol	NIST Webbook
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	2190.00	kPa	KDB
rinpol	968.00		NIST Webbook
rinpol	964.70		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	967.00		NIST Webbook

rinpol	974.50		NIST Webbook
rinpol	967.90		NIST Webbook
rinpol	971.30		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	968.42		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	969.13		NIST Webbook
rinpol	968.10		NIST Webbook
rinpol	968.53		NIST Webbook
rinpol	968.75		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	967.90		NIST Webbook
rinpol	968.93		NIST Webbook
rinpol	964.70		NIST Webbook
tb	439.70	K	KDB
tc	613.60	K	KDB
tf	185.00	K	KDB
vc	0.561	m ³ /kmol	KDB
zc	0.2408160		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.29	J/molxK	427.76	Joback Method
cpg	330.79	J/molxK	455.42	Joback Method
cpg	345.71	J/molxK	483.08	Joback Method
cpg	360.07	J/molxK	510.75	Joback Method
cpg	373.88	J/molxK	538.41	Joback Method
cpg	387.16	J/molxK	566.07	Joback Method
cpg	399.91	J/molxK	593.73	Joback Method
dvisc	0.0032190	Paxs	227.51	Joback Method

dvisc	0.0108083	Paxs	187.46	Joback Method
dvisc	0.0013777	Paxs	267.56	Joback Method
dvisc	0.0007355	Paxs	307.61	Joback Method
dvisc	0.0004537	Paxs	347.66	Joback Method
dvisc	0.0003093	Paxs	387.71	Joback Method
dvisc	0.0002265	Paxs	427.76	Joback Method
hvapt	38.70	kJ/mol	439.70	KDB
rfi	1.41360		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43717e+01
Coeff. B	-3.68827e+03
Coeff. C	-6.15080e+01
Temperature range (K), min.	323.38
Temperature range (K), max.	468.59

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.09681e+02
Coeff. B	-9.63118e+03
Coeff. C	-1.39251e+01
Coeff. D	8.22575e-06
Temperature range (K), min.	323.15
Temperature range (K), max.	613.60

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol102.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5881174&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=102>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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
mccv:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
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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