

Octane, 3,3-dimethyl-

Other names:	3,3-Dimethyloctane
Inchi:	InChI=1S/C10H22/c1-5-7-8-9-10(3,4)6-2/h5-9H2,1-4H3
InchiKey:	DBULLUBYDONGLT-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCC(C)(C)CC
Mol. weight [g/mol]:	142.28
CAS:	4110-44-5

Physical Properties

Property code	Value	Unit	Source
gf	36.16	kJ/mol	Joback Method
hf	-258.48	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	48.50	kJ/mol	NIST Webbook
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	935.50		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	935.50		NIST Webbook
rinpol	935.50		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	938.40		NIST Webbook
rinpol	934.40		NIST Webbook
rinpol	939.30		NIST Webbook
rinpol	936.00		NIST Webbook

rinpol	935.50		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	942.20		NIST Webbook
tb	429.15 ± 4.00	K	NIST Webbook
tb	434.35 ± 1.00	K	NIST Webbook
tc	597.50	K	Joback Method
tf	204.88	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/molxK	424.97	Joback Method
cpg	333.53	J/molxK	453.73	Joback Method
cpg	349.34	J/molxK	482.48	Joback Method
cpg	364.44	J/molxK	511.24	Joback Method
cpg	378.86	J/molxK	539.99	Joback Method
cpg	392.61	J/molxK	568.75	Joback Method
cpg	405.72	J/molxK	597.50	Joback Method
dvisc	0.0108562	Paxs	204.88	Joback Method
dvisc	0.0035911	Paxs	241.56	Joback Method
dvisc	0.0015903	Paxs	278.24	Joback Method
dvisc	0.0008514	Paxs	314.92	Joback Method
dvisc	0.0005192	Paxs	351.61	Joback Method
dvisc	0.0003477	Paxs	388.29	Joback Method
dvisc	0.0002495	Paxs	424.97	Joback Method

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41763e+01
Coeff. B	-3.56197e+03
Coeff. C	-6.16890e+01
Temperature range (K), min.	318.15
Temperature range (K), max.	463.50

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.01510e+02
Coeff. B	-9.09564e+03
Coeff. C	-1.27338e+01
Coeff. D	7.39631e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	612.10

Sources

KDB Vapor Pressure Data:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=110
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therc.org/files/research/kdb/mol/mol110.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4110445&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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