

Octane, 2,2-dimethyl-

Other names:	2,2-Dimethyloctane
Inchi:	InChI=1S/C10H22/c1-5-6-7-8-9-10(2,3)4/h5-9H2,1-4H3
InchiKey:	GPBUTTSWJNPYJL-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCCCC(C)(C)C
Mol. weight [g/mol]:	142.28
CAS:	15869-87-1

Physical Properties

Property code	Value	Unit	Source
af	0.4170		KDB
ap	354.150	K	KDB
gf	36.16	kJ/mol	Joback Method
hcg	6764.11	kJ/mol	KDB
hcn	6279.975	kJ/mol	KDB
hf	-258.48	kJ/mol	Joback Method
hfus	14.24	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
pc	2130.00	kPa	KDB
rinpol	918.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	922.80		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	918.70		NIST Webbook
rinpol	918.70		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.10		NIST Webbook
rinpol	914.90		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook

rinpol	916.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	922.80		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	917.60		NIST Webbook
rinpol	920.30		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	430.10	K	KDB
tc	602.00	K	KDB
tf	219.00	K	KDB
vc	0.580	m ³ /kmol	KDB
zc	0.2468170		KDB

Temperature Dependent Properties

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

dvisc	0.0015903	Paxs	278.24	Joback Method
dvisc	0.0035911	Paxs	241.56	Joback Method
hvapt	37.70	kJ/mol	430.10	KDB
rfi	1.40600		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43929e+01
Coeff. B	-3.68888e+03
Coeff. C	-5.26550e+01
Temperature range (K), min.	314.18
Temperature range (K), max.	458.85

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.24663e+01
Coeff. B	-7.79653e+03
Coeff. C	-8.31381e+00
Coeff. D	3.74626e-06
Temperature range (K), min.	225.00
Temperature range (K), max.	602.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermopedia.com/doc/thermophys/kdb/mol/mol104.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869871&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.thermopedia.com/doc/thermophys/kdb/hcprop/showprop.php?cmpid=104
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.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
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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