

Octane, 2,6-dimethyl-

Other names:	2,6-Dimethyloctane
Inchi:	InChI=1S/C10H22/c1-5-10(4)8-6-7-9(2)3/h9-10H,5-8H2,1-4H3
InchiKey:	ZALHPSXXQIPKTQ-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCC(C)CCCC(C)C
Mol. weight [g/mol]:	142.28
CAS:	2051-30-1

Physical Properties

Property code	Value	Unit	Source
af	0.4530		KDB
ap	351.150	K	KDB
gf	28.44	kJ/mol	Joback Method
hcg	6769.80	kJ/mol	KDB
hcn	6285.666	kJ/mol	KDB
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	49.30	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2150.00	kPa	KDB
rinpol	935.00		NIST Webbook
rinpol	933.30		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	934.70		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	932.00		NIST Webbook

rinpol	932.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	930.75		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	933.30		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	930.75		NIST Webbook
rinpol	935.12		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	935.12		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	931.50		NIST Webbook
rinpol	934.90		NIST Webbook
rinpol	934.90		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	930.80		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	938.00		NIST Webbook
ripol	921.00		NIST Webbook
ripol	921.00		NIST Webbook
tb	432.15 ± 1.50	K	NIST Webbook
tb	433.50	K	KDB
tb	432.90 ± 1.50	K	NIST Webbook
tb	433.40 ± 1.50	K	NIST Webbook
tb	431.65 ± 2.00	K	NIST Webbook
tb	432.65 ± 0.60	K	NIST Webbook
tb	431.65 ± 0.70	K	NIST Webbook
tb	431.65 ± 2.00	K	NIST Webbook
tc	603.10	K	KDB
tf	219.00	K	KDB
vc	0.576	m ³ /kmol	KDB
zc	0.2469650		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.93	J/mol×K	568.65	Joback Method

cpg	401.95	J/molxK	596.92	Joback Method
cpg	315.26	J/molxK	427.32	Joback Method
cpg	331.18	J/molxK	455.59	Joback Method
cpg	346.50	J/molxK	483.85	Joback Method
cpg	361.21	J/molxK	512.12	Joback Method
cpg	375.35	J/molxK	540.39	Joback Method
dvisc	0.0002171	Paxs	427.32	Joback Method
dvisc	0.0003059	Paxs	384.84	Joback Method
dvisc	0.0214146	Paxs	172.46	Joback Method
dvisc	0.0046771	Paxs	214.94	Joback Method
dvisc	0.0016877	Paxs	257.41	Joback Method
dvisc	0.0008129	Paxs	299.89	Joback Method
dvisc	0.0004693	Paxs	342.37	Joback Method
hvapt	38.20	kJ/mol	433.50	KDB
rfi	1.40840		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44779e+01
Coeff. B	-3.72529e+03
Coeff. C	-5.56960e+01
Temperature range (K), min.	318.22
Temperature range (K), max.	462.10

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.17854e+02
Coeff. B	-9.84801e+03
Coeff. C	-1.52027e+01
Coeff. D	9.76863e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	462.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=108
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051301&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=108
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	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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