

Octane, 2,4-dimethyl-

Other names:	2,4-dimethyloctane
Inchi:	InChI=1S/C10H22/c1-5-6-7-10(4)8-9(2)3/h9-10H,5-8H2,1-4H3
InchiKey:	IXAVTTRPEXFVVSX-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCC(C)CC(C)C
Mol. weight [g/mol]:	142.28
CAS:	4032-94-4

Physical Properties

Property code	Value	Unit	Source
af	0.4300		KDB
ap	353.150	K	KDB
gf	28.44	kJ/mol	Joback Method
hcg	6770.38	kJ/mol	KDB
hcn	6286.251	kJ/mol	KDB
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	48.50	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
pc	2140.00	kPa	KDB
rinpol	920.00		NIST Webbook
rinpol	915.50		NIST Webbook
rinpol	924.40		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	915.50		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	915.80		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	924.40		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.80		NIST Webbook

rinpol	916.80		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
tb	429.10	K	KDB
tb	429.05 ± 0.50	K	NIST Webbook
tc	599.40	K	KDB
tf	219.00	K	KDB
vc	0.566	m ³ /kmol	KDB
zc	0.2430390		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.95	J/mol×K	596.92	Joback Method
cpg	315.26	J/mol×K	427.32	Joback Method
cpg	331.18	J/mol×K	455.59	Joback Method
cpg	346.50	J/mol×K	483.85	Joback Method
cpg	361.21	J/mol×K	512.12	Joback Method
cpg	375.35	J/mol×K	540.39	Joback Method
cpg	388.93	J/mol×K	568.65	Joback Method
dvisc	0.0002171	Paxs	427.32	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
dvisc	0.0003059	Paxs	384.84	Joback Method
hvapt	42.40 ± 0.20	kJ/mol	358.00	NIST Webbook
hvapt	37.82	kJ/mol	429.10	KDB
hvapt	44.90 ± 0.20	kJ/mol	328.00	NIST Webbook
hvapt	43.60 ± 0.20	kJ/mol	343.00	NIST Webbook
rfi	1.40690		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41560e+01
Coeff. B	-3.45677e+03
Coeff. C	-6.66180e+01
Temperature range (K), min.	315.87
Temperature range (K), max.	457.45

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.05704e+02
Coeff. B	-9.29793e+03
Coeff. C	-1.33354e+01
Coeff. D	7.70166e-06
Temperature range (K), min.	316.15
Temperature range (K), max.	599.40

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=106
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4032944&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=106
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
hvac:	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
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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