Octane, 2,3-dimethyl-

Other names: 2,3-Dimethyloctane
Inchi: InChI=1S/C10H22/c1-5-6-7-8-10(4)9(2)3/h9-10H,5-8H2,1-4H3
InchiKey: YPMNDMUOGQJCLW-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCCCC(C)C(C)C
Mol. weight [g/mol]: 142.28
CAS: 7146-60-3

Physical Properties

Property code	Value	Unit	Source
af	0.4240		KDB
ap	348.150	K	KDB
gf	28.44	kJ/mol	Joback Method
hcg	6773.48	kJ/mol	KDB
hcn	6289.389	kJ/mol	KDB
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	48.10	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2190.00	kPa	KDB
rinpol	954.60		NIST Webbook
rinpol	955.30		NIST Webbook
rinpol	952.10		NIST Webbook
rinpol	951.80		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	961.90		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	957.30		NIST Webbook
rinpol	953.90		NIST Webbook
rinpol	958.80		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	959.00		NIST Webbook

rinpol	955.54		NIST Webbook
rinpol	955.88		NIST Webbook
rinpol	954.40		NIST Webbook
rinpol	955.21		NIST Webbook
rinpol	955.61		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	954.60		NIST Webbook
rinpol	954.65		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	954.00		NIST Webbook
tb	436.90 ± 0.50	K	NIST Webbook
tb	437.80 ± 0.50	K	NIST Webbook
tb	437.50	K	KDB
tb	437.46 ± 0.15	K	NIST Webbook
tc	613.20	K	KDB
tf	219.00	K	KDB
vc	0.567	m3/kmol	KDB
zc	0.2435500		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/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
dvisc	0.0002171	Pa×s	427.32	Joback Method
dvisc	0.0003059	Pa×s	384.84	Joback Method
dvisc	0.0214146	Pa×s	172.46	Joback Method
dvisc	0.0046771	Pa×s	214.94	Joback Method

dvisc	0.0016877	Pa×s	257.41	Joback Method
dvisc	0.0008129	Pa×s	299.89	Joback Method
dvisc	0.0004693	Pa×s	342.37	Joback Method
hvapt	38.20	kJ/mol	437.50	KDB
rfi	1.41270		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42414e+01
Coeff. B	-3.60471e+03
Coeff. C	-6.28790e+01
Temperature range (K), min.	321.21
Temperature range (K), max.	466.55

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.04960e+02
Coeff. B	-9.35083e+03
Coeff. C	-1.32274e+01
Coeff. D	7.68034e-06
Temperature range (K), min.	321.15
Temperature range (K), max.	613.20

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=105

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7146603&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=105

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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