Octane, 2,7-dimethyl-

Other names:	2,7-Dimethyloctane
	Diisoamyl
	Diisopentyl
Inchi:	InChI=1S/C10H22/c1-9(2)7-5-6-8-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	KEVMYFLMMDUPJE-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CC(C)CCCCC(C)C
Mol. weight [g/mol]:	142.28
CAS:	1072-16-8

Physical Properties

Property code	Value	Unit	Source
af	0.4380		KDB
ap	352.150	K	KDB
chl	-6747.11	kJ/mol	NIST Webbook
gf	28.44	kJ/mol	Joback Method
hcg	6767.62	kJ/mol	KDB
hcn	6283.490	kJ/mol	KDB
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	47.70	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2100.00	kPa	KDB
rinpol	928.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	927.80		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	928.50		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	930.40		NIST Webbook
rinpol	930.40		NIST Webbook

rinpol	928.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
tb	433.00	K	KDB
tc	602.90	K	KDB
tf	219.00	K	KDB
vc	0.590	m3/kmol	KDB
zc	0.2471660		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.93	J/mol×K	568.65	Joback Method
cpg	375.35	J/mol×K	540.39	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
cpl	301.70	J/mol×K	295.00	NIST Webbook
dvisc	0.0002171	Pa×s	427.32	Joback Method
dvisc	0.0004693	Pa×s	342.37	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
hvapt	45.20	kJ/mol	356.00	NIST Webbook
hvapt	38.24	kJ/mol	433.00	KDB
rfi	1.40620		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41298e+01
Coeff. B	-3.45264e+03

Coeff. C	-7.00330e+01
Temperature range (K), min.	319.46
Temperature range (K), max.	461.56

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08460e+02
Coeff. B	-9.52017e+03
Coeff. C	-1.37254e+01
Coeff. D	7.82701e-06
Temperature range (K), min.	319.15
Temperature range (K), max.	602.90

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/files/research/kdb/mol/mol109.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072168&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=109
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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