Octane, 3,6-dimethyl-

Other names: 3,6-Dimethyloctane
Inchi: InChI=1S/C10H22/c1-5-9(3)7-8-10(4)6-2/h9-10H,5-8H2,1-4H3
InchiKey: JEEQUUSFXYRPRK-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)CCC(C)CC
Mol. weight [g/mol]: 142.28
CAS: 15869-94-0

Physical Properties

Property code	Value	Unit	Source
gf	28.44	kJ/mol	Joback Method
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	47.30	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	940.60		NIST Webbook
rinpol	940.60		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	927.80		NIST Webbook
rinpol	927.80		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	948.30		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	944.00		NIST Webbook

rinpol	948.30		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method
tf	172.46	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	401.95	J/mol×K	596.92	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
dvisc	0.0003059	Pa×s	384.84	Joback Method
dvisc	0.0002171	Pa×s	427.32	Joback Method
rhol	746.60	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	738.90	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	731.10	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	723.30	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	715.50	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	707.60	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	699.60	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	691.50	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	683.30	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	674.90	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	746.60	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	738.90	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	731.20	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	723.50	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	715.70	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41976e+01
Coeff. B	-3.53609e+03
Coeff. C	-6.48190e+01
Temperature range (K), min.	319.03
Temperature range (K), max.	462.75

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.06372e+02
Coeff. B	-9.38170e+03
Coeff. C	-1.34381e+01
Coeff. D	7.80491e-06
Temperature range (K), min.	319.15
Temperature range (K), max.	608.30

Sources

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=113
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869940&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=113
Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:	https://www.doi.org/10.1021/je400274f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume