Octane, 2,5-dimethyl-

Other names: 2,5-Dimethyloctane
Inchi: InChI=1S/C10H22/c1-5-6-10(4)8-7-9(2)3/h9-10H,5-8H2,1-4H3
InchiKey: HOAAQUNESXYFDT-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCC(C)CCC(C)C
Mol. weight [g/mol]: 142.28
CAS: 15869-89-3

Physical Properties

Property code	Value	Unit	Source
af	0.4320		KDB
ap	350.150	K	KDB
gf	28.44	kJ/mol	Joback Method
hcg	6770.21	kJ/mol	KDB
hcn	6286.084	kJ/mol	KDB
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	49.00	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	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	932.60		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	922.30		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	932.60		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	921.80		NIST Webbook

rinpol	929.00		NIST Webbook
rinpol	922.40		NIST Webbook
rinpol	922.00		NIST Webbook
tb	429.15 ± 2.00	K	NIST Webbook
tb	430.15 ± 2.00	K	NIST Webbook
tb	430.00 ± 1.00	K	NIST Webbook
tb	431.70	K	KDB
tc	603.00	K	KDB
tf	219.00	K	KDB
vc	0.569	m3/kmol	KDB
zc	0.2440040		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	37.82	kJ/mol	431.70	KDB
rfi	1.40890		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42361e+01

Coeff. B	-3.54158e+03
Coeff. C	-6.34170e+01
Temperature range (K), min.	317.32
Temperature range (K), max.	460.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.07688e+02
Coeff. B	-9.39056e+03
Coeff. C	-1.36500e+01
Coeff. D	8.09315e-06
Temperature range (K), min.	317.15
Temperature range (K), max.	603.00

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=107

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869893&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=107

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

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

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