Pentane, 2,2,3-trimethyl-

Other names: (CH3)3CCH(CH3)CH2CH3
2,2,3-Trimethylpentane
Inchi: InChI=1S/C8H18/c1-6-7(2)8(3,4)5/h7H,6H2,1-5H3
InchiKey: XTDQDBVBDLYELW-UHFFFAOYSA-N
Formula: C8H18
SMILES: CCC(C)C(C)(C)C
Mol. weight [g/mol]: 114.23
CAS: 564-02-3

Physical Properties

Property code	Value	Unit	Source
af	0.2970		KDB
ap	343.950	K	KDB
chl	-5463.60 ± 1.40	kJ/mol	NIST Webbook
gf	17.12	kJ/mol	KDB
hcg	5463.59	kJ/mol	KDB
hcn	5067.452	kJ/mol	KDB
hf	-220.10 ± 1.50	kJ/mol	NIST Webbook
hf	-220.30	kJ/mol	KDB
hfl	-257.10 ± 1.50	kJ/mol	NIST Webbook
hfus	5.54	kJ/mol	Joback Method
hvap	36.91	kJ/mol	NIST Webbook
hvap	36.98	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	3.079		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	2730.00 ± 40.00	kPa	NIST Webbook
pc	2729.40 ± 40.53	kPa	NIST Webbook
pc	2730.00	kPa	KDB
rhoc	261.58 ± 4.57	kg/m3	NIST Webbook
rhoc	261.58 ± 4.57	kg/m3	NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	734.00		NIST Webbook

rinpol	734.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	734.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	737.30	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	734.00	NIST Webbook
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rinpol	737.00	NIST Webbook
rinpol	740.00	NIST Webbook
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rinpol	728.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	730.80	NIST Webbook
rinpol	732.00	NIST Webbook
rinpol	726.90	NIST Webbook
rinpol	726.90	NIST Webbook
rinpol	733.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	727.92	NIST Webbook
rinpol	729.78	NIST Webbook

rinpol	730.95		NIST Webbook
rinpol	728.57		NIST Webbook
rinpol	730.36		NIST Webbook
rinpol	731.52		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	732.00		NIST Webbook
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rinpol	737.00		NIST Webbook
rinpol	739.10		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	741.40		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	733.40		NIST Webbook
tb	382.99 ± 0.20	K	NIST Webbook
tb	383.15 ± 0.20	K	NIST Webbook
tb	383.80 ± 0.40	K	NIST Webbook
tb	383.25 ± 0.20	K	NIST Webbook
tb	382.97 ± 0.10	K	NIST Webbook
tb	383.20 ± 0.20	K	NIST Webbook
tb	383.00	K	KDB

tb	383.20	K	NIST Webbook
tb	383.00	K	NIST Webbook
tb	383.00 ± 0.20	K	NIST Webbook
tb	383.15 ± 0.30	K	NIST Webbook
tb	383.22 ± 0.50	K	NIST Webbook
tb	383.25 ± 0.50	K	NIST Webbook
tb	383.00 ± 0.15	K	NIST Webbook
tb	382.99 ± 0.05	K	NIST Webbook
tb	383.15 ± 0.50	K	NIST Webbook
tb	382.99 ± 0.02	K	NIST Webbook
tb	383.10 ± 0.15	K	NIST Webbook
tb	383.10 ± 0.15	K	NIST Webbook
tb	382.99 ± 0.05	K	NIST Webbook
tb	383.25 ± 0.60	K	NIST Webbook
tc	563.50	K	KDB
tc	563.50 ± 0.50	K	NIST Webbook
tc	563.43 ± 0.40	K	NIST Webbook
tf	160.83 ± 0.06	K	NIST Webbook
tf	159.85 ± 0.20	K	NIST Webbook
tf	160.88 ± 0.07	K	NIST Webbook
tf	160.89	K	KDB
tf	160.70 ± 0.30	K	NIST Webbook
tf	160.87 ± 0.20	K	NIST Webbook
tf	159.85 ± 0.50	K	NIST Webbook
tf	160.83 ± 0.30	K	NIST Webbook
tf	159.85 ± 0.50	K	NIST Webbook
tf	160.69 ± 0.02	K	NIST Webbook
tf	160.77 ± 0.20	K	NIST Webbook
tf	160.80 ± 0.10	K	NIST Webbook
vc	0.436	m3/kmol	KDB
vc	0.436	m3/kmol	NIST Webbook
zc	0.2540500		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.27	J/mol×K	557.09	Joback Method
cpg	233.00	J/mol×K	378.77	Joback Method
cpg	248.05	J/mol×K	408.49	Joback Method
cpg	262.39	J/mol×K	438.21	Joback Method
cpg	276.06	J/mol×K	467.93	Joback Method

cpg	289.08	J/mol×K	497.65	Joback Method
cpg	301.48	J/mol×K	527.37	Joback Method
dvisc	0.0002691	Pa×s	378.77	Joback Method
dvisc	0.0236666	Pa×s	167.34	Joback Method
dvisc	0.0058649	Pa×s	202.58	Joback Method
dvisc	0.0021975	Pa×s	237.82	Joback Method
dvisc	0.0010608	Pa×s	273.06	Joback Method
dvisc	0.0006049	Pa×s	308.29	Joback Method
dvisc	0.0003870	Pa×s	343.53	Joback Method
hvapt	31.94	kJ/mol	383.00	NIST Webbook
hvapt	32.01	kJ/mol	383.30	KDB
rfi	1.40066		298.15	KDB
rhol	716.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41543e+01
Coeff. B	-3.26180e+03
Coeff. C	-4.09360e+01
Temperature range (K), min.	276.16
Temperature range (K), max.	409.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.10435e+01
Coeff. B	-7.04729e+03
Coeff. C	-9.93298e+00
Coeff. D	7.20904e-06
Temperature range (K), min.	160.89
Temperature range (K), max.	563.50

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C564023&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=59
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=59
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=59

Legend

af:	Acentric Factor
ap:	Aniline Point
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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