Pentane, 3-methylene-

Other names:	(C2H5)2C=CH2
	1,1-DIETHYLETHENE
	1-Butene, 2-ethyl-
	2-Ethyl-1-butene
	2-ethylbut-1-ene
	3-METHYLENEPENTANE
Inchi:	InChI=1S/C6H12/c1-4-6(3)5-2/h3-5H2,1-2H3
InchiKey:	RYKZRKKEYSRDNF-UHFFFAOYSA-N
Formula:	C6H12
SMILES:	C=C(CC)CC
Mol. weight [g/mol]:	84.16
CAS:	760-21-4

Physical Properties

Property code	Value	Unit	Source
af	0.2670		KDB
gf	78.93	kJ/mol	Joback Method
hcg	3989.03	kJ/mol	KDB
hcn	3724.932	kJ/mol	KDB
hf	-56.07 ± 0.88	kJ/mol	NIST Webbook
hfl	-87.20 ± 0.80	kJ/mol	NIST Webbook
hfus	8.71	kJ/mol	Joback Method
hvap	31.00	kJ/mol	NIST Webbook
hvap	31.00	kJ/mol	NIST Webbook
ie	9.01	eV	NIST Webbook
ie	9.06 ± 0.01	eV	NIST Webbook
ie	9.06 ± 0.02	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
pc	3280.00	kPa	KDB
rinpol	584.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	592.10		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook

rinpol	608.00		NIST Webbook
rinpol	592.00		NIST Webbook
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rinpol	592.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	598.80		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	592.20		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	592.20		NIST Webbook
rinpol	598.80		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	587.00		NIST Webbook
tb	337.85 ± 0.30	K	NIST Webbook
tb	339.75 ± 1.00	K	NIST Webbook
tb	339.60 ± 0.60	K	NIST Webbook
tb	337.85 ± 0.30	K	NIST Webbook
tb	337.90	K	NIST Webbook
tb	338.10 ± 1.00	K	NIST Webbook
tb	340.65 ± 5.00	K	NIST Webbook
tb	337.84 ± 0.30	K	NIST Webbook
tb	337.95 ± 0.40	K	NIST Webbook
tb	338.15 ± 1.00	K	NIST Webbook
tb	339.60 ± 1.50	K	NIST Webbook
tb	337.80	K	KDB
tb	337.84 ± 0.30	K	NIST Webbook

tb	337.95 ± 0.60	K	NIST Webbook
tc	510.40	K	KDB
tf	142.00	K	KDB
tf	141.17 ± 0.30	K	NIST Webbook
tf	141.13 ± 0.20	K	NIST Webbook
vc	0.353	m3/kmol	KDB
zc	0.2732220		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.34	J/mol×K	475.05	Joback Method
cpg	145.82	J/mol×K	333.24	Joback Method
cpg	155.88	J/mol×K	361.60	Joback Method
cpg	165.55	J/mol×K	389.96	Joback Method
cpg	174.84	J/mol×K	418.33	Joback Method
cpg	183.77	J/mol×K	446.69	Joback Method
cpg	200.57	J/mol×K	503.41	Joback Method
hvapt	28.79	kJ/mol	337.80	KDB
rfi	1.39380		298.15	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40243e+01
Coeff. B	-2.84136e+03
Coeff. C	-3.57390e+01
Temperature range (K), min.	242.58
Temperature range (K), max.	361.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.84051e+01
Coeff. B	-5.53757e+03

Coeff. C	-6.49779e+00
Coeff. D	3.85159e-06
Temperature range (K), min.	141.61
Temperature range (K), max.	512.00

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/mol209.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C760214&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=209
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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