

2,3-Pentadiene

Other names:	1,3-DIMETHYLALLENE CH ₃ CH=C=CHCH ₃
Inchi:	InChI=1S/C5H8/c1-3-5-4-2/h3-4H,1-2H3
InchiKey:	PODAMDJNMAKAZ-UHFFFAOYSA-N
Formula:	C ₅ H ₈
SMILES:	CC=C=CC
Mol. weight [g/mol]:	68.12
CAS:	591-96-8

Physical Properties

Property code	Value	Unit	Source
af	0.2040		KDB
chg	-3243.90 ± 0.67	kJ/mol	NIST Webbook
gf	199.72	kJ/mol	Joback Method
hcg	3214.27	kJ/mol	KDB
hcn	3038.253	kJ/mol	KDB
hf	133.00 ± 0.71	kJ/mol	NIST Webbook
hfus	11.04	kJ/mol	Joback Method
hvap	29.50	kJ/mol	NIST Webbook
ie	9.13 ± 0.02	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.13	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.737		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4140.00	kPa	KDB
rinpol	530.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	556.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	532.00		NIST Webbook

rinpol	544.00		NIST Webbook
rinpol	556.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	531.10		NIST Webbook
rinpol	531.00		NIST Webbook
sg	329.11	J/molxK	NIST Webbook
sl	237.32	J/molxK	NIST Webbook
tb	321.35 ± 0.40	K	NIST Webbook
tb	321.40	K	KDB
tc	505.80	K	KDB
tf	147.50 ± 0.02	K	NIST Webbook
tf	147.46 ± 0.05	K	NIST Webbook
tf	147.43 ± 0.20	K	NIST Webbook
tf	147.43 ± 0.06	K	NIST Webbook
tf	148.00	K	KDB
tf	147.47 ± 0.04	K	NIST Webbook
tt	147.52 ± 0.05	K	NIST Webbook
tt	147.52 ± 0.05	K	NIST Webbook
vc	0.276	m3/kmol	KDB
zc	0.2712100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.68	J/molxK	505.54	Joback Method
cpg	141.56	J/molxK	474.82	Joback Method
cpg	135.19	J/molxK	444.11	Joback Method
cpg	128.58	J/molxK	413.39	Joback Method
cpg	121.71	J/molxK	382.67	Joback Method
cpg	114.59	J/molxK	351.95	Joback Method
cpg	107.19	J/molxK	321.23	Joback Method
cpl	152.34	J/molxK	298.15	NIST Webbook
hfust	6.13	kJ/mol	147.52	NIST Webbook
hfust	6.13	kJ/mol	147.50	NIST Webbook
hfust	6.13	kJ/mol	147.50	NIST Webbook
hfust	6.13	kJ/mol	147.52	NIST Webbook
hvapt	33.20	kJ/mol	230.00	NIST Webbook
hvapt	32.30	kJ/mol	246.00	NIST Webbook
hvapt	28.24	kJ/mol	321.40	KDB

hvapt	29.60	kJ/mol	310.00	NIST Webbook
hvapt	31.10	kJ/mol	294.00	NIST Webbook
rfi	1.42509		298.15	KDB
sfust	44.93	J/mol×K	147.52	NIST Webbook
sfust	44.93	J/mol×K	147.52	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41058e+01
Coeff. B	-2.69205e+03
Coeff. C	-3.76010e+01
Temperature range (K), min.	232.42
Temperature range (K), max.	343.71

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol363.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591968&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

af:	Acentric Factor
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpola:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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