

# Pentacosane

<b>Other names:</b>	n-Pentacosane
<b>Inchi:</b>	InChI=1S/C25H52/c1-3-5-7-9-11-13-15-17-19-21-23-25-24-22-20-18-16-14-12-10-8-6-4-2
<b>InchiKey:</b>	YKNWII LGEFFOPE-UHFFFAOYSA-N
<b>Formula:</b>	C25H52
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	352.68
<b>CAS:</b>	629-99-2

## Physical Properties

Property code	Value	Unit	Source
gf	159.62	kJ/mol	Joback Method
hf	-559.33	kJ/mol	Joback Method
hfus	55.53	kJ/mol	Solid liquid equilibria and purity determination for binary n-alkane + naphthalene systems
hsub	174.00 ± 10.00	kJ/mol	NIST Webbook
hvap	127.60 ± 0.80	kJ/mol	NIST Webbook
hvap	129.80 ± 2.90	kJ/mol	NIST Webbook
hvap	128.60 ± 2.20	kJ/mol	NIST Webbook
hvap	126.80	kJ/mol	NIST Webbook
log10ws	-10.29		Crippen Method
logp	9.998		Crippen Method
mcpvol	363.110	ml/mol	McGowan Method
pc	763.95	kPa	Joback Method
rinpol	394.59		NIST Webbook
rinpol	402.21		NIST Webbook
ss	671.10	J/molxK	NIST Webbook
tb	675.10	K	NIST Webbook
tc	944.85	K	Joback Method
tf	325.50 ± 2.00	K	NIST Webbook
tf	328.90 ± 1.00	K	NIST Webbook
tf	327.10 ± 1.00	K	NIST Webbook
tf	327.00 ± 3.00	K	NIST Webbook
tf	325.50 ± 3.00	K	NIST Webbook
tf	326.50 ± 0.50	K	NIST Webbook
tf	326.50 ± 0.60	K	NIST Webbook
tf	326.60 ± 0.20	K	NIST Webbook

tf	326.15 ± 3.00	K	NIST Webbook
tf	326.50 ± 0.60	K	NIST Webbook
tf	327.65 ± 2.00	K	NIST Webbook
tf	326.15 ± 2.00	K	NIST Webbook
tf	326.70 ± 0.30	K	NIST Webbook
tf	326.00 ± 0.10	K	NIST Webbook
tf	326.65	K	KDB
tf	327.20 ± 0.40	K	NIST Webbook
tf	326.90 ± 2.00	K	NIST Webbook
vc	1.435	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.43	J/mol×K	944.85	Joback Method
cpg	1174.90	J/mol×K	800.31	Joback Method
cpg	1218.47	J/mol×K	858.13	Joback Method
cpg	1197.21	J/mol×K	829.22	Joback Method
cpg	1238.74	J/mol×K	887.04	Joback Method
cpg	1258.04	J/mol×K	915.95	Joback Method
cpg	1151.50	J/mol×K	771.40	Joback Method
cpl	815.90	J/mol×K	333.00	NIST Webbook
cps	769.00	J/mol×K	294.50	NIST Webbook
dvisc	0.0020715	Paxs	371.51	Joback Method
dvisc	0.0001035	Paxs	638.10	Joback Method
dvisc	0.0000697	Paxs	704.75	Joback Method
dvisc	0.0006958	Paxs	438.16	Joback Method
dvisc	0.0000503	Paxs	771.40	Joback Method
dvisc	0.0001685	Paxs	571.45	Joback Method
dvisc	0.0003118	Paxs	504.81	Joback Method
hfust	79.39	kJ/mol	326.60	NIST Webbook
hfust	55.53	kJ/mol	325.90	NIST Webbook
hfust	57.80	kJ/mol	326.40	NIST Webbook
hfust	57.74	kJ/mol	326.70	NIST Webbook
hfust	26.07	kJ/mol	320.20	NIST Webbook
hfust	57.74	kJ/mol	326.70	NIST Webbook

hvapt	119.10	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure
hvapt	99.20	kJ/mol	566.00	NIST Webbook
hvapt	90.90 ± 5.70	kJ/mol	479.50	NIST Webbook
hvapt	97.60	kJ/mol	460.50	NIST Webbook
hvapt	126.00 ± 1.00	kJ/mol	415.50	NIST Webbook
hvapt	106.60	kJ/mol	422.00	NIST Webbook
hvapt	126.80	kJ/mol	298.15	Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography
pvap	0.09	kPa	461.98	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	8.02e-03	kPa	422.02	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	3.83e-03	kPa	411.78	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K

pvap	0.02	kPa	432.21	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	3.31e-04	kPa	381.69	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.03	kPa	442.34	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.05	kPa	452.24	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.05	kPa	452.25	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.09	kPa	461.95	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.09	kPa	461.98	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K

pvap	3.83e-03	kPa	411.75	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	1.78e-03	kPa	402.03	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	7.83e-04	kPa	391.91	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.03	kPa	442.33	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
sfust	243.10	J/molxK	326.60	NIST Webbook
sfust	176.76	J/molxK	326.70	NIST Webbook
sfust	81.42	J/molxK	320.20	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	5.22396e+02
Coeff. B	-3.82614e+04
Coeff. C	-7.31253e+01
Coeff. D	3.16722e-05
Temperature range (K), min.	355.15
Temperature range (K), max.	675.15

# Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C629992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C629992&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
A Comparison of Results by Correlation Gas Chromatography with Vapor Pressure and Vaporization Enthalpies of the n-Alkanes from 62 to 690 K and the Effects of Pressure on the Vaporization Enthalpies of n-Alkanes from 62 to 690 K	<a href="https://www.doi.org/10.1021/acs.jced.5b00444">https://www.doi.org/10.1021/acs.jced.5b00444</a>
Enthalpies of the n-Alkanes from 62 to 690 K and the Effects of Pressure on the Vaporization Enthalpies of n-Alkanes from 62 to 690 K	<a href="https://www.doi.org/10.1021/je0301747">https://www.doi.org/10.1021/je0301747</a>
Gas Chromatography and Vapor Pressure Temperature Range between 350 K and 460 K: KDB:	<a href="https://www.doi.org/10.1021/je050182i">https://www.doi.org/10.1021/je050182i</a>
Solid liquid equilibria and purity determination for binary n-alkane + K <sub>2</sub> Diuron systems	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
Crippen Method:	<a href="https://www.cheric.org/files/research/kdb/mol/mol25.mol">https://www.cheric.org/files/research/kdb/mol/mol25.mol</a>
Joback Method:	<a href="https://www.doi.org/10.1016/j.tca.2006.03.011">https://www.doi.org/10.1016/j.tca.2006.03.011</a>
	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=25">https://www.chemeo.com/doc/models/crippen_log10ws</a>
	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>ss:</b>	Solid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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