Pentacosane

Other names: n-Pentacosane
Inchi: 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
InchiKey: YKNWIILGEFFOPE-UHFFFAOYSA-N
Formula: C25H52
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 352.68
CAS: 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	126.80	kJ/mol	NIST Webbook
hvap	128.60 ± 2.20	kJ/mol	NIST Webbook
log10ws	-10.29		Crippen Method
logp	9.998		Crippen Method
mcvol	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/mol×K	NIST Webbook
tb	675.10	K	NIST Webbook
tc	944.85	K	Joback Method
tf	327.20 ± 0.40	K	NIST Webbook
tf	326.15 ± 3.00	K	NIST Webbook
tf	326.60 ± 0.20	K	NIST Webbook
tf	326.50 ± 0.60	K	NIST Webbook
tf	326.50 ± 0.50	K	NIST Webbook
tf	325.50 ± 3.00	K	NIST Webbook
tf	325.50 ± 2.00	K	NIST Webbook
tf	326.90 ± 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	326.65	K	KDB
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	326.50 ± 0.60	K	NIST Webbook
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.43	J/mol×K	944.85	Joback Method
cpg	1197.21	J/mol×K	829.22	Joback Method
cpg	1174.90	J/mol×K	800.31	Joback Method
cpg	1218.47	J/mol×K	858.13	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	0.0000697	Pa×s	704.75	Joback Method
dvisc	0.0001685	Pa×s	571.45	Joback Method
dvisc	0.0003118	Pa×s	504.81	Joback Method
dvisc	0.0001035	Pa×s	638.10	Joback Method
dvisc	0.0006958	Pa×s	438.16	Joback Method
dvisc	0.0020715	Pa×s	371.51	Joback Method
dvisc	0.0000503	Pa×s	771.40	Joback Method
hfust	57.74	kJ/mol	326.70	NIST Webbook
hfust	57.80	kJ/mol	326.40	NIST Webbook
hfust	55.53	kJ/mol	325.90	NIST Webbook
hfust	26.07	kJ/mol	320.20	NIST Webbook
hfust	79.39	kJ/mol	326.60	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	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	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

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	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	442.34	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	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	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
sfust	176.76	J/mol×K	326.70	NIST Webbook
sfust	81.42	J/mol×K	320.20	NIST Webbook
sfust	243.10	J/mol×K	326.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*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

Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K:	https://www.doi.org/10.1021/je050182i
Solid-liquid equilibria and purity determination for binary n-alkane + naphthalene systems:	https://www.doi.org/10.1016/j.tca.2006.03.011
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol25.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629992&Units=SI
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:	https://www.doi.org/10.1021/acs.jced.5b00444
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=25
Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C21 to C30 at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0301747
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume