Heptacosane

Other names: n-Heptacosane
Inchi: InChI=1S/C27H56/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-26-24-22-20-18-16-14-12-10-
InchiKey: BJQWYEJQWHSSCJ-UHFFFAOYSA-N
Formula: C27H56
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 380.73
CAS: 593-49-7

Physical Properties

Property code	Value	Unit	Source
gf	176.46	kJ/mol	Joback Method
hf	-600.61	kJ/mol	Joback Method
hfus	65.69	kJ/mol	Joback Method
hsub	196.00 ± 30.00	kJ/mol	NIST Webbook
hvap	75.70	kJ/mol	Joback Method
log10ws	-11.12		Crippen Method
logp	10.779		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	688.89	kPa	Joback Method
rinpol	429.45		NIST Webbook
rinpol	447.80		NIST Webbook
rinpol	426.00		NIST Webbook
rinpol	426.00		NIST Webbook
tb	817.16	K	Joback Method
tc	1000.84	K	Joback Method
tf	394.05	K	Joback Method
tt	332.00 ± 0.10	K	NIST Webbook
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1352.36	J/mol×K	909.00	Joback Method
cpg	1393.68	J/mol×K	970.23	Joback Method

cpg	1373.56	J/mol×K	939.61	Joback Method
cpg	1281.81	J/mol×K	817.16	Joback Method
cpg	1306.54	J/mol×K	847.77	Joback Method
cpg	1330.04	J/mol×K	878.39	Joback Method
cpg	1412.80	J/mol×K	1000.84	Joback Method
cps	828.00	J/mol×K	313.00	NIST Webbook
dvisc	0.0000526	Pa×s	746.64	Joback Method
dvisc	0.0000379	Pa×s	817.16	Joback Method
dvisc	0.0001282	Pa×s	605.61	Joback Method
dvisc	0.0002384	Pa×s	535.09	Joback Method
dvisc	0.0005356	Pa×s	464.57	Joback Method
dvisc	0.0016072	Pa×s	394.05	Joback Method
dvisc	0.0000784	Pa×s	676.12	Joback Method
hfust	59.05	kJ/mol	332.10	NIST Webbook
hfust	26.28	kJ/mol	325.40	NIST Webbook
hfust	2.26	kJ/mol	318.00	NIST Webbook
hfust	59.05	kJ/mol	332.10	NIST Webbook
hfust	62.80	kJ/mol	331.60	NIST Webbook
hvapt	116.90 ± 3.00	kJ/mol	421.00	NIST Webbook
hvapt	104.30	kJ/mol	584.00	NIST Webbook
hvapt	135.60	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
hvapt	132.00 ± 1.00	kJ/mol	421.00	NIST Webbook
hvapt	94.20	kJ/mol	539.00	NIST Webbook
pvap	0.04	kPa	462.27	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.04	kPa	462.27	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	452.27	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	0.01	kPa	442.18	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	5.56e-03	kPa	432.03	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	2.72e-03	kPa	421.95	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	2.69e-03	kPa	421.93	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	1.30e-03	kPa	411.81	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	1.29e-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	5.90e-04	kPa	401.69	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	5.92e-04	kPa	401.68	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
sfust	177.82	J/mol×K	332.10	NIST Webbook
sfust	80.75	J/mol×K	325.40	NIST Webbook
sfust	7.11	J/mol×K	318.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	543.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.45690e+02
Coeff. B	-3.16699e+04
Coeff. C	-4.62242e+01
Coeff. D	1.44570e-05
Temperature range (K), min.	473.15
Temperature range (K), max.	695.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=27
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol27.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C593497&Units=SI

Legend

cpg:	Ideal gas 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume