Nonacosane

Other names: n-nonacosane
Inchi: InChI=1S/C29H60/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-28-26-24-22-20-18-16-14-
InchiKey: IGGUPRCHHJZPBS-UHFFFAOYSA-N
Formula: C29H60
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 408.79
CAS: 630-03-5

Physical Properties

Property code	Value	Unit	Source
gf	193.30	kJ/mol	Joback Method
hf	-641.89	kJ/mol	Joback Method
hfus	70.87	kJ/mol	Joback Method
hvap	147.10	kJ/mol	NIST Webbook
log10ws	-11.96		Crippen Method
logp	11.559		Crippen Method
mcvol	419.470	ml/mol	McGowan Method
pc	624.38	kPa	Joback Method
rinpol	475.30		NIST Webbook
rinpol	454.90		NIST Webbook
rinpol	454.90		NIST Webbook
tb	714.00	K	NIST Webbook
tc	1060.53	K	Joback Method
tf	335.70 ± 3.00	K	NIST Webbook
tf	336.00 ± 4.00	K	NIST Webbook
tf	338.00 ± 1.00	K	NIST Webbook
tf	336.60 ± 0.40	K	NIST Webbook
tf	336.70 ± 0.80	K	NIST Webbook
tf	337.00 ± 2.00	K	NIST Webbook
tf	334.20 ± 2.00	K	NIST Webbook
tf	336.50 ± 0.60	K	NIST Webbook
tf	337.00 ± 2.00	K	NIST Webbook
tf	337.00 ± 1.00	K	NIST Webbook
vc	1.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1553.04	J/mol×K	1060.53	Joback Method
cpg	1414.73	J/mol×K	862.92	Joback Method
cpg	1489.65	J/mol×K	961.72	Joback Method
cpg	1511.96	J/mol×K	994.66	Joback Method
cpg	1533.07	J/mol×K	1027.59	Joback Method
cpg	1466.05	J/mol×K	928.79	Joback Method
cpg	1441.10	J/mol×K	895.85	Joback Method
dvisc	0.0000282	Pa×s	862.92	Joback Method
dvisc	0.0000393	Pa×s	788.53	Joback Method
dvisc	0.0000588	Pa×s	714.14	Joback Method
dvisc	0.0000965	Pa×s	639.75	Joback Method
dvisc	0.0001803	Pa×s	565.37	Joback Method
dvisc	0.0012311	Pa×s	416.59	Joback Method
dvisc	0.0004073	Pa×s	490.98	Joback Method
hfust	66.11	kJ/mol	336.60	NIST Webbook
hfust	29.71	kJ/mol	331.40	NIST Webbook
hfust	66.11	kJ/mol	336.60	NIST Webbook
hvapt	137.00 ± 3.00	kJ/mol	440.00	NIST Webbook
hvapt	112.50	kJ/mol	437.00	NIST Webbook
hvapt	137.10 ± 3.00	kJ/mol	439.50	NIST Webbook
hvapt	147.10	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	109.00	kJ/mol	601.00	NIST Webbook
pvap	2.06e-03	kPa	432.12	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K

pvap	9.71e-04	kPa	422.10	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	8.19e-03	kPa	452.23	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	8.24e-03	kPa	452.20	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	4.17e-03	kPa	442.19	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	4.21e-03	kPa	442.17	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
pvap	9.70e-04	kPa	422.10	Experimental Vapor Pressures of Six n-Alkanes (C21, C23, C25, C27, C29, C30) in the Temperature Range between 350 K and 460 K
sfust	196.43	J/mol×K	336.60	NIST Webbook
sfust	89.65	J/mol×K	331.40	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	559.20	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas 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
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

vc: Critical Volume