

Hexadecane, 4-undecyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C27H56/c1-4-7-9-11-13-15-17-19-21-23-26-27(24-6-3)25-22-20-18-16-14-12-1

CWDPPKDZKLJVBY-UHFFFAOYSA-N

C27H56

CCCCCCCCCCCC(CCC)CCCCCCCCCCCC

380.73

Physical Properties

Property code	Value	Unit	Source
gf	174.02	kJ/mol	Joback Method
hf	-605.89	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-10.88		Crippen Method
logp	10.635		Crippen Method
mcvol	391.290	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2574.00		NIST Webbook
tb	816.72	K	Joback Method
tc	1000.04	K	Joback Method
tf	379.05	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.19	J/mol×K	816.72	Joback Method
cpg	1393.80	J/mol×K	969.49	Joback Method
cpg	1373.74	J/mol×K	938.93	Joback Method
cpg	1352.60	J/mol×K	908.38	Joback Method
cpg	1330.33	J/mol×K	877.83	Joback Method
cpg	1306.88	J/mol×K	847.27	Joback Method
cpg	1412.85	J/mol×K	1000.04	Joback Method
dvisc	0.0000347	Pa×s	816.72	Joback Method
dvisc	0.0000492	Pa×s	743.77	Joback Method

dvisc	0.0000750	Pa×s	670.83	Joback Method
dvisc	0.0001269	Pa×s	597.88	Joback Method
dvisc	0.0002484	Pa×s	524.94	Joback Method
dvisc	0.0006041	Pa×s	451.99	Joback Method
dvisc	0.0020683	Pa×s	379.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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