

Hexadecane, 6-undecyl

Inchi:	InChI=1S/C27H56/c1-4-7-10-12-14-16-18-20-23-26-27(24-21-9-6-3)25-22-19-17-15-13-1
InchiKey:	TXFJLBXOUSFPDJ-UHFFFAOYSA-N
Formula:	C27H56
SMILES:	CCCCCCCCCCCC(CCCCC)CCCCCCCCC
Mol. weight [g/mol]:	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
mvol	391.290	ml/mol	McGowan Method
pc	691.79	kPa	Joback Method
rinpol	2548.00		NIST Webbook
tb	816.72	K	Joback Method
tc	1000.04	K	Joback Method
tf	379.05	K	Joback Method
vc	1.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.19	J/molxK	816.72	Joback Method
cpg	1306.88	J/molxK	847.27	Joback Method
cpg	1330.33	J/molxK	877.83	Joback Method
cpg	1352.60	J/molxK	908.38	Joback Method
cpg	1373.74	J/molxK	938.93	Joback Method
cpg	1393.80	J/molxK	969.49	Joback Method
cpg	1412.85	J/molxK	1000.04	Joback Method
dvisc	0.0020683	Paxs	379.05	Joback Method
dvisc	0.0006041	Paxs	451.99	Joback Method

dvisc	0.0002484	Paxs	524.94	Joback Method
dvisc	0.0001269	Paxs	597.88	Joback Method
dvisc	0.0000750	Paxs	670.83	Joback Method
dvisc	0.0000492	Paxs	743.77	Joback Method
dvisc	0.0000347	Paxs	816.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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