

Hexadecane, 6-propyl

Inchi:	InChI=1S/C19H40/c1-4-7-9-10-11-12-13-15-18-19(16-6-3)17-14-8-5-2/h19H,4-18H2,1-3H
InchiKey:	FKDHMZSFJFQVOE-UHFFFAOYSA-N
Formula:	C19H40
SMILES:	CCCCCCCCCCC(CCC)CCCC
Mol. weight [g/mol]:	268.52

Physical Properties

Property code	Value	Unit	Source
gf	106.66	kJ/mol	Joback Method
hf	-440.77	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.514		Crippen Method
mvol	278.570	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	633.68	K	Joback Method
tc	794.96	K	Joback Method
tf	288.89	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.70	J/molxK	633.68	Joback Method
cpg	877.35	J/molxK	768.08	Joback Method
cpg	859.82	J/molxK	741.20	Joback Method
cpg	841.51	J/molxK	714.32	Joback Method
cpg	822.41	J/molxK	687.44	Joback Method
cpg	802.48	J/molxK	660.56	Joback Method
cpg	894.13	J/molxK	794.96	Joback Method
dvisc	0.0001019	Paxs	633.68	Joback Method

dvisc	0.0001427	Paxs	576.22	Joback Method
dvisc	0.0002152	Paxs	518.75	Joback Method
dvisc	0.0003595	Paxs	461.29	Joback Method
dvisc	0.0006952	Paxs	403.82	Joback Method
dvisc	0.0016729	Paxs	346.36	Joback Method
dvisc	0.0057089	Paxs	288.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47938&Units=SI

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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