

Hexadecane, 5-methyl

Inchi:	InChI=1S/C17H36/c1-4-6-8-9-10-11-12-13-14-16-17(3)15-7-5-2/h17H,4-16H2,1-3H3
InchiKey:	LNFKUZITRWJITR-UHFFFAOYSA-N
Formula:	C17H36
SMILES:	CCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	240.47

Physical Properties

Property code	Value	Unit	Source
gf	89.82	kJ/mol	Joback Method
hf	-399.49	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.734		Crippen Method
mcvol	250.390	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1651.00		NIST Webbook
tb	587.92	K	Joback Method
tc	748.86	K	Joback Method
tf	266.35	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.18	J/molxK	587.92	Joback Method
cpg	687.14	J/molxK	614.74	Joback Method
cpg	706.30	J/molxK	641.57	Joback Method
cpg	724.69	J/molxK	668.39	Joback Method
cpg	742.33	J/molxK	695.21	Joback Method
cpg	759.24	J/molxK	722.04	Joback Method
cpg	775.45	J/molxK	748.86	Joback Method

dvisc	0.0070198	Paxs	266.35	Joback Method
dvisc	0.0020606	Paxs	319.94	Joback Method
dvisc	0.0008598	Paxs	373.54	Joback Method
dvisc	0.0004468	Paxs	427.13	Joback Method
dvisc	0.0002686	Paxs	480.73	Joback Method
dvisc	0.0001789	Paxs	534.33	Joback Method
dvisc	0.0001283	Paxs	587.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R47817&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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