

Hexadecane, 6-ethyl

Inchi:	InChI=1S/C18H38/c1-4-7-9-10-11-12-13-15-17-18(6-3)16-14-8-5-2/h18H,4-17H2,1-3H3
InchiKey:	XKCYQWUTQACFFN-UHFFFAOYSA-N
Formula:	C18H38
SMILES:	CCCCCCCCCCC(CC)CCCC
Mol. weight [g/mol]:	254.49

Physical Properties

Property code	Value	Unit	Source
gf	98.24	kJ/mol	Joback Method
hf	-420.13	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	7.124		Crippen Method
mvol	264.480	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	610.80	K	Joback Method
tc	771.74	K	Joback Method
tf	277.62	K	Joback Method
vc	1.038	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.79	J/molxK	610.80	Joback Method
cpg	817.70	J/molxK	744.91	Joback Method
cpg	800.46	J/molxK	718.09	Joback Method
cpg	782.48	J/molxK	691.27	Joback Method
cpg	763.72	J/molxK	664.45	Joback Method
cpg	744.17	J/molxK	637.62	Joback Method
cpg	834.20	J/molxK	771.74	Joback Method
dvisc	0.0001146	Paxs	610.80	Joback Method

dvisc	0.0001602	Paxs	555.27	Joback Method
dvisc	0.0002411	Paxs	499.74	Joback Method
dvisc	0.0004019	Paxs	444.21	Joback Method
dvisc	0.0007754	Paxs	388.68	Joback Method
dvisc	0.0018624	Paxs	333.15	Joback Method
dvisc	0.0063506	Paxs	277.62	Joback Method

Sources

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=R46776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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