Hexadecane, 3-methyl-

Other names: 3-Methylhexadecane
Inchi: InChI=1S/C17H36/c1-4-6-7-8-9-10-11-12-13-14-15-16-17(3)5-2/h17H,4-16H2,1-3H3
InchiKey: WWPCLIMUTNKTDY-UHFFFAOYSA-N
Formula: C17H36
SMILES: CCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 240.47
CAS: 6418-43-5

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	1677.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1673.00		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	775.45	J/mol×K	748.86	Joback Method

cpg	759.24	J/mol×K	722.04	Joback Method
cpg	742.33	J/mol×K	695.21	Joback Method
cpg	724.69	J/mol×K	668.39	Joback Method
cpg	706.30	J/mol×K	641.57	Joback Method
cpg	687.14	J/mol×K	614.74	Joback Method
cpg	667.18	J/mol×K	587.92	Joback Method
dvisc	0.0070198	Pa×s	266.35	Joback Method
dvisc	0.0001283	Pa×s	587.92	Joback Method
dvisc	0.0001789	Pa×s	534.33	Joback Method
dvisc	0.0002686	Pa×s	480.73	Joback Method
dvisc	0.0004468	Pa×s	427.13	Joback Method
dvisc	0.0008598	Pa×s	373.54	Joback Method
dvisc	0.0020606	Pa×s	319.94	Joback Method
hvapt	63.40	kJ/mol	497.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42805e+01
Coeff. B	-4.32094e+03
Coeff. C	-1.23950e+02
Temperature range (K), min.	432.74
Temperature range (K), max.	605.71

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=C6418435&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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