Hexadecane, 4-methyl-

Other names: 4-Methylhexadecane
Inchi: InChI=1S/C17H36/c1-4-6-7-8-9-10-11-12-13-14-16-17(3)15-5-2/h17H,4-16H2,1-3H3
InchiKey: OREPYGSHKSWUCK-UHFFFAOYSA-N
Formula: C17H36
SMILES: CCCCCCCCCCCCC(C)CCC
Mol. weight [g/mol]: 240.47
CAS: 25117-26-4

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	1659.90		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1659.00		NIST Webbook
ripol	1655.00		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/mol×K	587.92	Joback Method
cpg	687.14	J/mol×K	614.74	Joback Method
cpg	706.30	J/mol×K	641.57	Joback Method
cpg	724.69	J/mol×K	668.39	Joback Method

cpg	742.33	J/mol×K	695.21	Joback Method
cpg	759.24	J/mol×K	722.04	Joback Method
cpg	775.45	J/mol×K	748.86	Joback Method
dvisc	0.0070198	Pa×s	266.35	Joback Method
dvisc	0.0020606	Pa×s	319.94	Joback Method
dvisc	0.0008598	Pa×s	373.54	Joback Method
dvisc	0.0004468	Pa×s	427.13	Joback Method
dvisc	0.0002686	Pa×s	480.73	Joback Method
dvisc	0.0001789	Pa×s	534.33	Joback Method
dvisc	0.0001283	Pa×s	587.92	Joback Method
hvapt	58.70	kJ/mol	493.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69584e+01
Coeff. B	-6.97978e+03
Coeff. C	-1.85600e+00
Temperature range (K), min.	420.54
Temperature range (K), max.	601.14

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117264&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

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume