Heptadecane, 3-methyl-

Other names:	3-Methylheptadecane
	Hexadecane, 2-ethyl
Inchi:	InChI=1S/C18H38/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18(3)5-2/h18H,4-17H2,1-3H3
InchiKey:	HPDKJRSKBCPMIY-UHFFFAOYSA-N
Formula:	C18H38
SMILES:	CCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]:	254.49
CAS:	6418-44-6

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
mcvol	264.480	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1771.20		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1773.20		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1768.40		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1773.20		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1770.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1769.20		NIST Webbook

tb	610.80	K	Joback Method
tc	771.74	K	Joback Method
tf	267.00 ± 2.00	K	NIST Webbook
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.79	J/mol×K	610.80	Joback Method
cpg	744.17	J/mol×K	637.62	Joback Method
cpg	763.72	J/mol×K	664.45	Joback Method
cpg	782.48	J/mol×K	691.27	Joback Method
cpg	800.46	J/mol×K	718.09	Joback Method
cpg	817.70	J/mol×K	744.91	Joback Method
cpg	834.20	J/mol×K	771.74	Joback Method
dvisc	0.0063506	Pa×s	277.62	Joback Method
dvisc	0.0018624	Pa×s	333.15	Joback Method
dvisc	0.0007754	Pa×s	388.68	Joback Method
dvisc	0.0004019	Pa×s	444.21	Joback Method
dvisc	0.0002411	Pa×s	499.74	Joback Method
dvisc	0.0001602	Pa×s	555.27	Joback Method
dvisc	0.0001146	Pa×s	610.80	Joback Method
hvapt	65.60	kJ/mol	512.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42537e+01
Coeff. B	-4.39662e+03
Coeff. C	-1.29850e+02
Temperature range (K), min.	444.66
Temperature range (K), max.	621.52

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6418446&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
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
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