Octadecane, 2-methyl-

Other names: 2-Methyloctadecane
Inchi: InChI=1S/C19H40/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(2)3/h19H,4-18H2,1-3H
InchiKey: KVQVGSDBGJXNGV-UHFFFAOYSA-N
Formula: C19H40
SMILES: CCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 268.52
CAS: 1560-88-9

Physical Properties

Property code	Value	Unit	Source
gf	106.66	kJ/mol	Joback Method
hf	-440.77	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.514		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1865.30		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1860.40		NIST Webbook
rinpol	1863.20		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1865.30		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1864.00		NIST Webbook
ripol	1861.70		NIST Webbook
ripol	1861.70		NIST Webbook
tb	633.68	K	Joback Method
tc	794.96	K	Joback Method
tf	284.40 ± 1.50	K	NIST Webbook
tf	286.00 ± 2.00	K	NIST Webbook
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.13	J/mol×K	794.96	Joback Method
cpg	781.70	J/mol×K	633.68	Joback Method
cpg	802.48	J/mol×K	660.56	Joback Method
cpg	822.41	J/mol×K	687.44	Joback Method
cpg	841.51	J/mol×K	714.32	Joback Method
cpg	859.82	J/mol×K	741.20	Joback Method
cpg	877.35	J/mol×K	768.08	Joback Method
dvisc	0.0001019	Pa×s	633.68	Joback Method
dvisc	0.0057089	Pa×s	288.89	Joback Method
dvisc	0.0016729	Pa×s	346.36	Joback Method
dvisc	0.0006952	Pa×s	403.82	Joback Method
dvisc	0.0003595	Pa×s	461.29	Joback Method
dvisc	0.0002152	Pa×s	518.75	Joback Method
dvisc	0.0001427	Pa×s	576.22	Joback Method
hvapt	67.50	kJ/mol	523.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42026e+01
Coeff. B	-4.44327e+03
Coeff. C	-1.35550e+02
Temperature range (K), min.	454.86
Temperature range (K), max.	635.29

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1560889&Units=SI

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