

Heptadecane, 2-methyl-

Other names:	2-Methylheptadecane
Inchi:	InChI=1S/C18H38/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2)3/h18H,4-17H2,1-3H3
InchiKey:	RJWUMFHQJJBOD-UHFFFAOYSA-N
Formula:	C18H38
SMILES:	CCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]:	254.49
CAS:	1560-89-0

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	1766.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1765.30		NIST Webbook
tb	584.20	K	NIST Webbook
tc	771.74	K	Joback Method
tf	278.00 ± 3.00	K	NIST Webbook
tf	278.00 ± 3.00	K	NIST Webbook
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	744.17	J/molxK	637.62	Joback Method
cpg	763.72	J/molxK	664.45	Joback Method
cpg	782.48	J/molxK	691.27	Joback Method
cpg	800.46	J/molxK	718.09	Joback Method
cpg	817.70	J/molxK	744.91	Joback Method
cpg	834.20	J/molxK	771.74	Joback Method
dvisc	0.0063506	Paxs	277.62	Joback Method
dvisc	0.0018624	Paxs	333.15	Joback Method
dvisc	0.0007754	Paxs	388.68	Joback Method
dvisc	0.0004019	Paxs	444.21	Joback Method
dvisc	0.0002411	Paxs	499.74	Joback Method
dvisc	0.0001602	Paxs	555.27	Joback Method
dvisc	0.0001146	Paxs	610.80	Joback Method
hvapt	67.80	kJ/mol	511.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	451.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43154e+01
Coeff. B	-4.40588e+03
Coeff. C	-1.29850e+02
Temperature range (K), min.	443.93
Temperature range (K), max.	619.18

Sources

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=C1560890&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/ci9903071

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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