2-Methylhexadec-1-ene

Other names: 1-Hexadecene, 2-methyl
2-Methyl-1-hexadecene
Inchi: InChI=1S/C17H34/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17(2)3/h2,4-16H2,1,3H3
InchiKey: DRLMBCPWFSTWNY-UHFFFAOYSA-N
Formula: C17H34
SMILES: C=C(C)CCCCCCCCCCCCCC
Mol. weight [g/mol]: 238.45
CAS: 61868-19-7

Physical Properties

Property code	Value	Unit	Source
gf	171.55	kJ/mol	Joback Method
hf	-278.57	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.654		Crippen Method
mcvol	246.090	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	584.92	K	Joback Method
tc	747.64	K	Joback Method
tf	265.63	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.09	J/mol×K	584.92	Joback Method
cpg	664.51	J/mol×K	612.04	Joback Method
cpg	683.14	J/mol×K	639.16	Joback Method

cpg	701.00	J/mol×K	666.28	Joback Method
cpg	718.11	J/mol×K	693.40	Joback Method
cpg	734.50	J/mol×K	720.52	Joback Method
cpg	750.20	J/mol×K	747.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54737e+01
Coeff. B	-5.13527e+03
Coeff. C	-9.11500e+01
Temperature range (K), min.	429.30
Temperature range (K), max.	596.48

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61868197&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

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

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