5-Methylnonadecane

Other names: Hexadecane, 2-butyl
Inchi: InChI=1S/C20H42/c1-4-6-8-9-10-11-12-13-14-15-16-17-19-20(3)18-7-5-2/h20H,4-19H2,1
InchiKey: ZFWCHSBHHWYGCK-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 282.55
CAS: 57160-72-2

Physical Properties

Property code	Value	Unit	Source
af	0.8164		Cheméo Relay (1.0)
gf	115.08	kJ/mol	Joback Method
hf	-466.47	kJ/mol	Cheméo Relay (1.0)
hfus	44.03	kJ/mol	Joback Method
hvap	95.79	kJ/mol	Cheméo Relay (1.0)
ie	9.72	eV	Cheméo Relay (1.0)
log10ws	-8.57		Cheméo Relay (1.0)
logp	7.904		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
tb	575.50	K	Cheméo Relay (1.0)
tc	744.05	K	Cheméo Relay (1.0)
tf	269.22	K	Cheméo Relay (1.0)
vc	1.152	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.17	J/mol×K	791.58	Joback Method
cpg	955.21	J/mol×K	818.58	Joback Method
cpg	862.00	J/mol×K	683.56	Joback Method
cpg	882.29	J/mol×K	710.57	Joback Method
cpg	901.73	J/mol×K	737.57	Joback Method
cpg	920.35	J/mol×K	764.58	Joback Method

cpg	840.82	J/mol×K	656.56	Joback Method
dvisc	0.0006199	Pa×s	418.96	Joback Method
dvisc	0.0014944	Pa×s	359.56	Joback Method
dvisc	0.0051032	Pa×s	300.16	Joback Method
dvisc	0.0003200	Pa×s	478.36	Joback Method
dvisc	0.0001911	Pa×s	537.76	Joback Method
dvisc	0.0001265	Pa×s	597.16	Joback Method
dvisc	0.0000902	Pa×s	656.56	Joback Method
hvapt	69.10	kJ/mol	535.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.82211e+01
Coeff. B	-8.27437e+03
Coeff. C	-8.86000e-01
Temperature range (K), min.	462.28
Temperature range (K), max.	641.83

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57160722&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume