Hexadecane, 5-butyl-

Other names: 5-Butylhexadecane
5-n-Butylhexadecane
Inchi: InChI=1S/C20H42/c1-4-7-10-11-12-13-14-15-16-19-20(17-8-5-2)18-9-6-3/h20H,4-19H2,1
InchiKey: WCYRXBXHFUHSAH-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCCCCCCCCC(CCCC)CCCC
Mol. weight [g/mol]: 282.55
CAS: 6912-07-8

Physical Properties

Property code	Value	Unit	Source
gf	115.08	kJ/mol	Joback Method
hf	-461.41	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.904		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	656.56	K	Joback Method
tc	818.58	K	Joback Method
tf	261.60 ± 2.00	K	NIST Webbook
tf	261.55	K	NIST Webbook
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.82	J/mol×K	656.56	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	938.17	J/mol×K	791.58	Joback Method
cpg	955.21	J/mol×K	818.58	Joback Method
dvisc	0.0051032	Pa×s	300.16	Joback Method
dvisc	0.0014944	Pa×s	359.56	Joback Method
dvisc	0.0006199	Pa×s	418.96	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	77.30	kJ/mol	440.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.06257e+01
Coeff. B	-9.29803e+03
Temperature range (K), min.	457.17
Temperature range (K), max.	607.15

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=C6912078&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume