Naphthalene, 1-butyl-

Other names:	1-Butylnaphthalene
	1-Naphthyl-1-butane
	1-n-Butylnaphthalene
	ALPHA-BUTYLNAPHTHALENE
	«alpha»-Butylnaphthalene
	Â«alphaÂ»-Butylnaphthalene
Inchi:	InChI=1S/C14H16/c1-2-3-7-12-9-6-10-13-8-4-5-11-14(12)13/h4-6,8-11H,2-3,7H2,1H3
InchiKey:	URGSMJLDEFDWNX-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	CCCCc1cccc2ccccc12
Mol. weight [g/mol]:	184.28
CAS:	1634-09-9

Physical Properties

Property code	Value	Unit	Source
af	0.5330		KDB
chl	-7427.00	kJ/mol	NIST Webbook
gf	276.43	kJ/mol	Joback Method
hf	83.84	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	51.34	kJ/mol	Joback Method
ie	7.76	eV	NIST Webbook
log10ws	-4.92		Crippen Method
logp	4.182		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2500.00	kPa	KDB
rinpol	1555.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	562.60	K	KDB
tc	781.50	K	KDB
tf	207.00 ± 5.00	K	NIST Webbook
tf	250.00 ± 4.00	K	NIST Webbook
tf	253.39 ± 0.20	K	NIST Webbook
tf	253.00	K	KDB
vc	0.633	m3/kmol	KDB

zc	0.2437370	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.98	J/mol×K	570.36	Joback Method
cpg	406.66	J/mol×K	607.36	Joback Method
cpg	422.22	J/mol×K	644.36	Joback Method
cpg	436.74	J/mol×K	681.35	Joback Method
cpg	450.29	J/mol×K	718.35	Joback Method
cpg	462.95	J/mol×K	755.35	Joback Method
cpg	474.78	J/mol×K	792.35	Joback Method
dvisc	0.0017208	Pa×s	319.18	Joback Method
dvisc	0.0010679	Pa×s	361.04	Joback Method
dvisc	0.0007318	Pa×s	402.91	Joback Method
dvisc	0.0005385	Pa×s	444.77	Joback Method
dvisc	0.0004177	Pa×s	486.63	Joback Method
dvisc	0.0003373	Pa×s	528.50	Joback Method
dvisc	0.0002810	Pa×s	570.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	9.41357e+00
Coeff. B	-1.49039e+03
Coeff. C	-2.49195e+02
Temperature range (K), min.	412.51
Temperature range (K), max.	612.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46266e+02
Coeff. B	-1.44257e+04
Coeff. C	-1.86294e+01

Coeff. D	6.55933e-06
Temperature range (K), min.	253.43
Temperature range (K), max.	792.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1634099&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=794
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol794.mol

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility