Naphthalene, 1-hexyl-

Other names: 1-N-HEXYLNAPHTHALENE
Inchi: InChI=1S/C16H20/c1-2-3-4-5-9-14-11-8-12-15-10-6-7-13-16(14)15/h6-8,10-13H,2-5,9H2
InchiKey: XRJWGFXUIIXRNM-UHFFFAOYSA-N
Formula: C16H20
SMILES: CCCCCCc1cccc2ccccc12
Mol. weight [g/mol]: 212.33
CAS: 2876-53-1

Physical Properties

Property code	Value	Unit	Source
gf	293.27	kJ/mol	Joback Method
hf	42.56	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.963		Crippen Method
mcvol	193.080	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	616.12	K	Joback Method
tc	830.41	K	Joback Method
tf	341.72	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.95	J/mol×K	616.12	Joback Method
cpg	507.63	J/mol×K	651.83	Joback Method
cpg	524.20	J/mol×K	687.55	Joback Method
cpg	539.72	J/mol×K	723.26	Joback Method
cpg	554.26	J/mol×K	758.98	Joback Method
cpg	567.91	J/mol×K	794.69	Joback Method
cpg	580.72	J/mol×K	830.41	Joback Method
dvisc	0.0017615	Pa×s	341.72	Joback Method

dvisc	0.0010486	Pa×s	387.45	Joback Method
dvisc	0.0006965	Pa×s	433.19	Joback Method
dvisc	0.0005002	Pa×s	478.92	Joback Method
dvisc	0.0003806	Pa×s	524.65	Joback Method
dvisc	0.0003026	Pa×s	570.39	Joback Method
dvisc	0.0002489	Pa×s	616.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.19659e+02
Coeff. B	-1.40519e+04
Coeff. C	-1.45455e+01
Coeff. D	4.24082e-06
Temperature range (K), min.	255.15
Temperature range (K), max.	813.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876531&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=802
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/mol802.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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