

Naphthalene, 7-butyl-1-hexyl-

Other names:	7-Butyl-1-hexylnaphthalene
Inchi:	InChI=1S/C20H28/c1-3-5-7-8-11-18-12-9-13-19-15-14-17(10-6-4-2)16-20(18)19/h9,12-16
InchiKey:	LPEFBGSLSJQKAH-UHFFFAOYSA-N
Formula:	C20H28
SMILES:	CCCCCCc1cccc2ccc(CCCC)cc12
Mol. weight [g/mol]:	268.44
CAS:	55000-55-0

Physical Properties

Property code	Value	Unit	Source
gf	317.32	kJ/mol	Joback Method
hf	-51.47	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.305		Crippen Method
mcvol	249.440	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
tb	712.62	K	Joback Method
tc	915.83	K	Joback Method
tf	399.32	K	Joback Method
vc	0.970	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.03	J/molxK	712.62	Joback Method
cpg	724.75	J/molxK	746.49	Joback Method
cpg	742.42	J/molxK	780.36	Joback Method
cpg	759.09	J/molxK	814.22	Joback Method
cpg	774.83	J/molxK	848.09	Joback Method
cpg	789.71	J/molxK	881.96	Joback Method
cpg	803.79	J/molxK	915.83	Joback Method
dvisc	0.0013226	Paxs	399.32	Joback Method

dvisc	0.0007792	Paxs	451.54	Joback Method
dvisc	0.0005123	Paxs	503.75	Joback Method
dvisc	0.0003644	Paxs	555.97	Joback Method
dvisc	0.0002748	Paxs	608.19	Joback Method
dvisc	0.0002167	Paxs	660.40	Joback Method
dvisc	0.0001770	Paxs	712.62	Joback Method
hvapt	78.10	kJ/mol	449.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.12368e+01
Coeff. B	-1.11831e+04
Coeff. C	5.31860e+01
Temperature range (K), min.	480.64
Temperature range (K), max.	649.04

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55000550&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/ci9903071
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

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

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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