

Naphthalene, 6-butyl-7-hexyl-1,2,3,4-tetrahydro-

Other names: 1,2,3,4-Tetrahydro-6-butyl-7-hexylnaphthalene

6-Butyl-7-hexyl-1,2,3,4-tetrahydronaphthalene

Inchi: InChI=1S/C20H32/c1-3-5-7-8-12-18-16-20-14-10-9-13-19(20)15-17(18)11-6-4-2/h15-16H

InchiKey: QKAUPJCSSOTPHK-UHFFFAOYSA-N

Formula: C20H32

SMILES: CCCCCc1cc2c(cc1CCCC)CCCC2

Mol. weight [g/mol]: 272.47

CAS: 66538-96-3

Physical Properties

Property code	Value	Unit	Source
gf	257.40	kJ/mol	Joback Method
hf	-167.03	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.031		Crippen Method
mvol	258.040	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
tb	714.30	K	Joback Method
tc	914.72	K	Joback Method
tf	397.80	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.38	J/molxK	714.30	Joback Method
cpg	775.85	J/molxK	747.70	Joback Method
cpg	795.20	J/molxK	781.11	Joback Method
cpg	813.48	J/molxK	814.51	Joback Method
cpg	830.75	J/molxK	847.91	Joback Method
cpg	847.07	J/molxK	881.32	Joback Method
cpg	862.52	J/molxK	914.72	Joback Method

dvisc	0.0015060	Paxs	397.80	Joback Method
dvisc	0.0008314	Paxs	450.55	Joback Method
dvisc	0.0005199	Paxs	503.30	Joback Method
dvisc	0.0003554	Paxs	556.05	Joback Method
dvisc	0.0002595	Paxs	608.80	Joback Method
dvisc	0.0001992	Paxs	661.55	Joback Method
dvisc	0.0001590	Paxs	714.30	Joback Method
hvapt	78.10	kJ/mol	444.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.96579e+01
Coeff. B	-9.99456e+03
Coeff. C	4.08820e+01
Temperature range (K), min.	475.09
Temperature range (K), max.	655.78

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66538963&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/72-710-3/Naphthalene-6-butyl-7-hexyl-1-2-3-4-tetrahydro.pdf>

Generated by Cheméo on 2024-04-19 02:11:22.761192658 +0000 UTC m=+15781931.681769974.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.