6-BUTYL-7-HEXYL-1,2,3,4-TETRAHYDRONAPHTH

Other names: 1,2,3,4-Tetrahydro-6-butyl-7-hexylnaphthalene
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: CCCCCCc1cc2c(cc1CCCC)CCCC2
Mol. weight [g/mol]: 272.48
CAS: 66538-96-3

Physical Properties

Property code	Value	Unit	Source
hfus	35.39	kJ/mol	Joback Method
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-7.45		Cheméo Relay (1.0)
logp	6.031		Crippen Method
mcvol	258.040	ml/mol	McGowan Method
tb	630.56	K	Cheméo Relay (1.0)
tf	288.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.38	J/mol×K	714.30	Joback Method
cpg	775.85	J/mol×K	747.70	Joback Method
cpg	795.20	J/mol×K	781.11	Joback Method
cpg	813.48	J/mol×K	814.51	Joback Method
cpg	830.75	J/mol×K	847.91	Joback Method
cpg	847.07	J/mol×K	881.32	Joback Method
cpg	862.52	J/mol×K	914.72	Joback Method
dvisc	0.0015060	Pa×s	397.80	Joback Method
dvisc	0.0008314	Pa×s	450.55	Joback Method
dvisc	0.0005199	Pa×s	503.30	Joback Method
dvisc	0.0003554	Pa×s	556.05	Joback Method
dvisc	0.0002595	Pa×s	608.80	Joback Method
dvisc	0.0001992	Pa×s	661.55	Joback Method

dvisc	0.0001590	Pa×s	714.30	Joback Method
hvapt	78.10	kJ/mol	444.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66538963&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point