

Naphthalene, 5-butyl-1,2,3,4-tetrahydro-

Other names:	5-Butyl-tetralin
Inchi:	InChI=1S/C14H20/c1-2-3-7-12-9-6-10-13-8-4-5-11-14(12)13/h6,9-10H,2-5,7-8,11H2,1H3
InchiKey:	HLZHYZXDQGEU-UHFFFAOYSA-N
Formula:	C14H20
SMILES:	CCCCc1cccc2c1CCCC2
Mol. weight [g/mol]:	188.31
CAS:	66325-42-6

Physical Properties

Property code	Value	Unit	Source
chl	-7782.00	kJ/mol	NIST Webbook
gf	216.51	kJ/mol	Joback Method
hf	-31.72	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.908		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	553.06 ± 0.30	K	NIST Webbook
tc	789.82	K	Joback Method
tf	224.00 ± 2.00	K	NIST Webbook
vc	0.661	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.38	J/mol×K	572.04	Joback Method
cpg	448.35	J/mol×K	608.34	Joback Method
cpg	466.15	J/mol×K	644.63	Joback Method
cpg	482.84	J/mol×K	680.93	Joback Method
cpg	498.48	J/mol×K	717.22	Joback Method

cpg	513.14	J/mol×K	753.52	Joback Method
cpg	526.89	J/mol×K	789.82	Joback Method
dvisc	0.0022322	Paxs	317.66	Joback Method
dvisc	0.0012779	Paxs	360.06	Joback Method
dvisc	0.0008228	Paxs	402.45	Joback Method
dvisc	0.0005761	Paxs	444.85	Joback Method
dvisc	0.0004292	Paxs	487.25	Joback Method
dvisc	0.0003352	Paxs	529.64	Joback Method
dvisc	0.0002716	Paxs	572.04	Joback Method

Sources

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=C66325426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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