

Naphthalene, 2-(1,1-dimethylethyl)-1,2,3,4-tetrahydro-

Other names:	2-tert-Butyl-1,2,3,4-Tetrahydronaphthalene 2-tert-Butyltetralin Naphthalene, 1,2,3,4-tetrahydro-2-(1,1-dimethylethyl)
Inchi:	InChI=1S/C14H20/c1-14(2,3)13-9-8-11-6-4-5-7-12(11)10-13/h4-7,13H,8-10H2,1-3H3
InchiKey:	FCXYHCYNCWKCOS-UHFFFAOYSA-N
Formula:	C14H20
SMILES:	CC(C)(C)C1CCc2ccccc2C1
Mol. weight [g/mol]:	188.31
CAS:	42044-22-4

Physical Properties

Property code	Value	Unit	Source
gf	221.27	kJ/mol	Joback Method
hf	-49.34	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.838		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	559.16	K	Joback Method
tc	789.80	K	Joback Method
tf	303.32	K	Joback Method
vc	0.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.97	J/mol×K	559.16	Joback Method
cpg	454.08	J/mol×K	597.60	Joback Method
cpg	473.68	J/mol×K	636.04	Joback Method
cpg	491.85	J/mol×K	674.48	Joback Method

cpg	508.71	J/mol×K	712.92	Joback Method
cpg	524.35	J/mol×K	751.36	Joback Method
cpg	538.87	J/mol×K	789.80	Joback Method
dvisc	0.0029253	Paxs	303.32	Joback Method
dvisc	0.0015589	Paxs	345.96	Joback Method
dvisc	0.0009538	Paxs	388.60	Joback Method
dvisc	0.0006432	Paxs	431.24	Joback Method
dvisc	0.0004655	Paxs	473.88	Joback Method
dvisc	0.0003554	Paxs	516.52	Joback Method
dvisc	0.0002828	Paxs	559.16	Joback Method

Sources

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=C42044224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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