

Naphthalene, 2-phenyl-

Other names:	(.beta.-naphthyl)benzene .beta.-phenylnaphthalene 2-phenylnaphthalene NSC 407592 «beta»-Phenylnaphthalene
Inchi:	InChI=1S/C16H12/c1-2-6-13(7-3-1)16-11-10-14-8-4-5-9-15(14)12-16/h1-12H
InchiKey:	TURIHPLQSRVWHU-UHFFFAOYSA-N
Formula:	C16H12
SMILES:	c1ccc(-c2ccc3ccccc3c2)cc1
Mol. weight [g/mol]:	204.27
CAS:	612-94-2

Physical Properties

Property code	Value	Unit	Source
gf	405.68	kJ/mol	Joback Method
hf	279.09	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Phase transition thermodynamics of phenyl and biphenyl naphthalenes
hsub	107.60 ± 0.60	kJ/mol	NIST Webbook
hvap	58.06	kJ/mol	Joback Method
ie	7.75	eV	NIST Webbook
log10ws	-5.88		Crippen Method
logp	4.507		Crippen Method
mcvol	169.320	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1949.90		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	343.50		NIST Webbook
rinpol	330.45		NIST Webbook
rinpol	330.85		NIST Webbook
rinpol	330.76		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	331.25		NIST Webbook
rinpol	333.90		NIST Webbook
rinpol	333.90		NIST Webbook
rinpol	330.83		NIST Webbook

rinpol	331.00		NIST Webbook
rinpol	331.20		NIST Webbook
rinpol	331.07		NIST Webbook
rinpol	330.29		NIST Webbook
rinpol	330.73		NIST Webbook
rinpol	332.64		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	330.20		NIST Webbook
rinpol	355.43		NIST Webbook
rinpol	326.13		NIST Webbook
rinpol	326.50		NIST Webbook
rinpol	330.50		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	326.39		NIST Webbook
rinpol	329.88		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	329.78		NIST Webbook
rinpol	331.10		NIST Webbook
rinpol	332.60		NIST Webbook
rinpol	326.51		NIST Webbook
rinpol	331.98		NIST Webbook
rinpol	332.17		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	331.10		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	343.50		NIST Webbook
rinpol	1958.50		NIST Webbook
rinpol	331.20		NIST Webbook
rinpol	332.59		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	330.20		NIST Webbook
rinpol	330.50		NIST Webbook
rinpol	331.10		NIST Webbook
rinpol	331.25		NIST Webbook
rinpol	330.50		NIST Webbook
rinpol	330.64		NIST Webbook
tb	618.70	K	NIST Webbook
tc	905.43	K	Joback Method
tf	375.00 ± 3.00	K	NIST Webbook
tf	374.40 ± 2.00	K	NIST Webbook
tf	374.90 ± 1.00	K	NIST Webbook
tf	375.20 ± 1.50	K	NIST Webbook

tt	374.77	K	Thermodynamic properties of 1-phenylnaphthalene and 2-phenylnaphthalene
vc	0.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.55	J/mol×K	861.65	Joback Method
cpg	470.95	J/mol×K	817.88	Joback Method
cpg	458.29	J/mol×K	774.11	Joback Method
cpg	444.42	J/mol×K	730.34	Joback Method
cpg	429.21	J/mol×K	686.57	Joback Method
cpg	412.52	J/mol×K	642.80	Joback Method
cpg	493.25	J/mol×K	905.43	Joback Method
dvisc	0.0015202	Pa×s	368.14	Joback Method
dvisc	0.0002560	Pa×s	642.80	Joback Method
dvisc	0.0003074	Pa×s	597.02	Joback Method
dvisc	0.0003805	Pa×s	551.25	Joback Method
dvisc	0.0004897	Pa×s	505.47	Joback Method
dvisc	0.0006626	Pa×s	459.69	Joback Method
dvisc	0.0009586	Pa×s	413.92	Joback Method
hfust	17.90	kJ/mol	373.50	NIST Webbook
hsubt	106.60 ± 0.40	kJ/mol	343.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.70	K	0.70	NIST Webbook

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=C612942&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Phase transition thermodynamics of
phenyl and biphenyl naphthalenes:
Thermodynamic properties of
1-phenylnaphthalene and
2-phenylnaphthalene:

<https://www.doi.org/10.1016/j.jct.2008.04.010>

<https://www.doi.org/10.1016/j.jct.2014.01.006>

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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