Naphthalene, 1-phenyl-

Other names: 1-Phenylnaphthalene
Inchi: InChI=1S/C16H12/c1-2-7-13(8-3-1)16-12-6-10-14-9-4-5-11-15(14)16/h1-12H
InchiKey: IYDMICQAKLQHLA-UHFFFAOYSA-N
Formula: C16H12
SMILES: c1ccc(-c2cccc3ccccc23)cc1
Mol. weight [g/mol]: 204.27
CAS: 605-02-7

Physical Properties

Property code	Value	Unit	Source
gf	405.68	kJ/mol	Joback Method
hf	279.09	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	81.10 ± 1.80	kJ/mol	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	315.11		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	1827.20		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	326.40		NIST Webbook
rinpol	326.40		NIST Webbook
rinpol	312.59		NIST Webbook
rinpol	312.59		NIST Webbook
rinpol	312.91		NIST Webbook
rinpol	313.30		NIST Webbook
rinpol	309.20		NIST Webbook
rinpol	309.20		NIST Webbook
rinpol	1841.70		NIST Webbook

rinpol	313.05		NIST Webbook
rinpol	313.60		NIST Webbook
rinpol	313.96		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	312.74		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	312.20		NIST Webbook
rinpol	315.21		NIST Webbook
rinpol	312.60		NIST Webbook
rinpol	312.60		NIST Webbook
rinpol	310.02		NIST Webbook
rinpol	312.59		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	313.90		NIST Webbook
rinpol	314.23		NIST Webbook
rinpol	314.35		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	1834.60		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	1841.70		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	1858.20		NIST Webbook
rinpol	315.19		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	311.39		NIST Webbook
tb	607.20	K	NIST Webbook
tb	597.70	K	NIST Webbook
tc	905.43	K	Joback Method
tf	368.14	K	Joback Method
tt	297.47	K	Thermodynamic properties of 1-phenylnaphthalene and 2-phenylnaphthalene
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.52	J/mol×K	642.80	Joback Method
cpg	429.21	J/mol×K	686.57	Joback Method

cpg	444.42	J/mol×K	730.34	Joback Method
cpg	458.29	J/mol×K	774.11	Joback Method
cpg	470.95	J/mol×K	817.88	Joback Method
cpg	482.55	J/mol×K	861.65	Joback Method
cpg	493.25	J/mol×K	905.43	Joback Method
dvisc	0.0009586	Pa×s	413.92	Joback Method
dvisc	0.0015202	Pa×s	368.14	Joback Method
dvisc	0.0006626	Pa×s	459.69	Joback Method
dvisc	0.0004897	Pa×s	505.47	Joback Method
dvisc	0.0003805	Pa×s	551.25	Joback Method
dvisc	0.0003074	Pa×s	597.02	Joback Method
dvisc	0.0002560	Pa×s	642.80	Joback Method
hsubt	88.60	kJ/mol	383.00	NIST Webbook
hvapt	81.00	kJ/mol	298.15	Phase transition thermodynamics of phenyl and biphenyl naphthalenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.07690e+01
Coeff. B	-7.50975e+03
Coeff. C	-8.59360e+01
Temperature range (K), min.	452.60
Temperature range (K), max.	571.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.66243e+01
Coeff. B	-1.29035e+04
Coeff. C	-1.11976e+01
Coeff. D	2.70396e-06
Temperature range (K), min.	318.15
Temperature range (K), max.	849.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C605027&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol801.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=801
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic properties of 1-phenylnaphthalene and 2-phenylnaphthalene:	https://www.doi.org/10.1016/j.jct.2014.01.006
Phase transition thermodynamics of phenyl and biphenyl naphthalenes:	https://www.doi.org/10.1016/j.jct.2008.04.010
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

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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