Naphthalene, 1,4-dimethyl-

Other names: 1,4-Dimethylnaphthalene
1,4-Dimethylnapthalene
Inchi: InChI=1S/C12H12/c1-9-7-8-10(2)12-6-4-3-5-11(9)12/h3-8H,1-2H3
InchiKey: APQSQLNWAIULLK-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1ccc(C)c2ccccc12
Mol. weight [g/mol]: 156.22
CAS: 571-58-4

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
ea	0.25 ± 0.08	eV	NIST Webbook
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfus	10.60	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hvap	47.55	kJ/mol	Joback Method
ie	7.78 ± 0.03	eV	NIST Webbook
ie	7.82 ± 0.03	eV	NIST Webbook
log10ws	-4.14		Estimated Solubility Method
log10ws	-4.14		Aqueous Solubility Prediction Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	1409.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1442.80		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1425.90		NIST Webbook
rinpol	1419.00		NIST Webbook

rinpol	1397.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1424.20	NIST Webbook
rinpol	1436.30	NIST Webbook
rinpol	1443.20	NIST Webbook
rinpol	1424.20	NIST Webbook
rinpol	1436.30	NIST Webbook
rinpol	1443.20	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1447.00	NIST Webbook
rinpol	1399.47	NIST Webbook
rinpol	1411.24	NIST Webbook
rinpol	1419.17	NIST Webbook
rinpol	1436.73	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1426.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1443.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	246.51	NIST Webbook
rinpol	1410.60	NIST Webbook
rinpol	246.55	NIST Webbook
rinpol	246.42	NIST Webbook
rinpol	243.02	NIST Webbook
rinpol	245.70	NIST Webbook
rinpol	246.20	NIST Webbook
rinpol	247.15	NIST Webbook
rinpol	246.03	NIST Webbook
rinpol	243.57	NIST Webbook
rinpol	245.40	NIST Webbook
rinpol	246.50	NIST Webbook
rinpol	243.60	NIST Webbook
rinpol	247.02	NIST Webbook
rinpol	243.98	NIST Webbook
rinpol	246.00	NIST Webbook
rinpol	246.30	NIST Webbook
rinpol	246.51	NIST Webbook
rinpol	245.70	NIST Webbook
rinpol	1443.00	NIST Webbook
rinpol	1410.60	NIST Webbook

rinpol	1442.80		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	243.57		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
tb	536.00 ± 4.00	K	NIST Webbook
tb	541.60 ± 1.00	K	NIST Webbook
tb	538.30	K	Critical properties of some alkylnaphthalenes
tb	540.50	K	KDB
tb	537.00 ± 4.00	K	NIST Webbook
tb	539.00 ± 5.00	K	NIST Webbook
tc	776.80	K	KDB
tf	280.73 ± 0.15	K	NIST Webbook
tf	280.81 ± 0.06	K	NIST Webbook
tf	279.00 ± 4.00	K	NIST Webbook
tf	289.45 ± 0.70	K	NIST Webbook
tf	281.02 ± 0.06	K	NIST Webbook
tf	289.00 ± 6.00	K	NIST Webbook
tf	289.00 ± 6.00	K	NIST Webbook
tf	253.00 ± 30.00	K	NIST Webbook
tf	281.00 ± 0.15	K	NIST Webbook
tf	279.20 ± 5.00	K	NIST Webbook
tf	279.90 ± 0.20	K	NIST Webbook
tf	280.75	K	Aqueous Solubility Prediction Method
tf	281.00	K	KDB
tf	271.00 ± 5.00	K	NIST Webbook
vc	0.521	m3/kmol	KDB
zc	0.2430380		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.06	J/mol×K	722.55	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cpg	296.31	J/mol×K	529.58	Joback Method
cpg	349.89	J/mol×K	683.95	Joback Method
cpg	371.48	J/mol×K	761.14	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method

dvisc	0.0002960	Pa×s	529.58	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
hfust	10.60	kJ/mol	279.90	NIST Webbook
hfust	10.60	kJ/mol	279.20	NIST Webbook
hfust	10.60	kJ/mol	279.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	536.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53305e+01
Coeff. B	-5.54175e+03
Coeff. C	-2.42690e+01
Temperature range (K), min.	392.66
Temperature range (K), max.	577.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.54930e+01
Coeff. B	-1.06126e+04
Coeff. C	-9.85429e+00
Coeff. D	2.89872e-06
Temperature range (K), min.	283.15
Temperature range (K), max.	776.78

Sources

Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene isomers:	https://www.doi.org/10.1021/je700088n
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Critical properties of some alkylnaphthalenes:	https://www.doi.org/10.1016/j.fluid.2013.08.041
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C571584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=772
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol772.mol

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility