1,5-DIMETHYLNAPHTHALENE

Other names:	1,5-Dimethlnapthalene
	naphthalene, 1,5-dimethyl-
Inchi:	InChI=1S/C12H12/c1-9-5-3-8-12-10(2)6-4-7-11(9)12/h3-8H,1-2H3
InchiKey:	SDDBCEWUYXVGCQ-UHFFFAOYSA-N
Formula:	C12H12
SMILES:	Cc1cccc2c(C)cccc12
Mol. weight [g/mol]:	156.23
CAS:	571-61-9

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
gf	249.96	kJ/mol	Joback Method
hf	88.59	kJ/mol	Cheméo Relay (1.0)
hfus	20.00	kJ/mol	Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers
hvap	67.02	kJ/mol	Cheméo Relay (1.0)
ie	7.85 ± 0.03	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
log10ws	-4.74		Aqueous Solubility Prediction Method
log10ws	-4.68		Estimated Solubility Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	246.51		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1438.40		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	246.80		NIST Webbook
rinpol	246.80		NIST Webbook
rinpol	247.62		NIST Webbook
rinpol	245.00		NIST Webbook
rinpol	247.30		NIST Webbook
rinpol	245.60		NIST Webbook
rinpol	244.98		NIST Webbook

rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1445.80		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1428.30		NIST Webbook
rinpol	1439.80		NIST Webbook
rinpol	1446.40		NIST Webbook
rinpol	1428.30		NIST Webbook
rinpol	1439.80		NIST Webbook
rinpol	1446.40		NIST Webbook
rinpol	1398.40		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	246.92		NIST Webbook
rinpol	1438.40		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1420.70		NIST Webbook
rinpol	247.62		NIST Webbook
rinpol	244.98		NIST Webbook
rinpol	247.00		NIST Webbook
rinpol	245.83		NIST Webbook
rinpol	246.70		NIST Webbook
ripol	2048.00		NIST Webbook
tb	538.00 ± 6.00	K	NIST Webbook
tb	538.20	K	KDB
tb	538.20	K	NIST Webbook
tb	542.30 ± 2.00	K	NIST Webbook
tc	773.50	K	KDB
tf	355.15 ± 0.50	K	NIST Webbook
tf	354.00 ± 4.00	K	NIST Webbook
tf	351.00 ± 2.00	K	NIST Webbook
tf	355.00	K	KDB
vc	0.521	m3/kmol	KDB
zc	0.2440750		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.31	J/mol×K	529.58	Joback Method
cpg	311.16	J/mol×K	568.17	Joback Method
cpg	325.00	J/mol×K	606.77	Joback Method
cpg	337.89	J/mol×K	645.36	Joback Method
cpg	349.89	J/mol×K	683.95	Joback Method
cpg	361.06	J/mol×K	722.55	Joback Method
cpg	371.48	J/mol×K	761.14	Joback Method
dvisc	0.0008686	Pa×s	345.90	Joback Method
dvisc	0.0012561	Pa×s	309.16	Joback Method
dvisc	0.0006448	Pa×s	382.63	Joback Method
dvisc	0.0005043	Pa×s	419.37	Joback Method
dvisc	0.0004103	Pa×s	456.11	Joback Method
dvisc	0.0003443	Pa×s	492.84	Joback Method
dvisc	0.0002960	Pa×s	529.58	Joback Method
hfust	20.00	kJ/mol	355.20	NIST Webbook
hvapt	64.10	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46150e+01
Coeff. B	-4.58671e+03
Coeff. C	-7.93770e+01
Temperature range (K), min.	399.51
Temperature range (K), max.	572.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.13472e+02
Coeff. B	-1.76632e+04
Coeff. C	-2.85522e+01

Coeff. D	1.21170e-05
Temperature range (K), min.	423.15
Temperature range (K), max.	773.47

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibria of Binary Mixtures of Dimethylnaphthalene Isomers:	https://www.doi.org/10.1021/je700088n
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=773
KDB:	https://www.cheric.org/files/research/kdb/mol/mol773.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C571619&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility