Naphthalene, 1,3-dimethyl-

Other names: 1,3-Dimethylnaphthalene
Inchi: InChI=1S/C12H12/c1-9-7-10(2)12-6-4-3-5-11(12)8-9/h3-8H,1-2H3
InchiKey: QHJMFSMPSZREIF-UHFFFAOYSA-N
Formula: C12H12
SMILES: Cc1cc(C)c2ccccc2c1
Mol. weight [g/mol]: 156.22
CAS: 575-41-7

Physical Properties

Property code	Value	Unit	Source
af	0.4430		KDB
gf	249.96	kJ/mol	Joback Method
hf	113.65	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
ie	7.86 ± 0.03	eV	NIST Webbook
log10ws	-4.29		Estimated Solubility Method
log10ws	-4.29		Aqueous Solubility Prediction Method
logp	3.457		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3010.00	kPa	KDB
rinpol	1423.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1405.30		NIST Webbook
rinpol	1416.50		NIST Webbook
rinpol	1422.30		NIST Webbook
rinpol	1405.30		NIST Webbook
rinpol	1416.50		NIST Webbook
rinpol	1422.30		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1397.00		NIST Webbook

rinpol	1424.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1415.40		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	242.99		NIST Webbook
rinpol	240.25		NIST Webbook
rinpol	243.42		NIST Webbook
rinpol	242.38		NIST Webbook
rinpol	1402.30		NIST Webbook
rinpol	243.31		NIST Webbook
rinpol	242.90		NIST Webbook
rinpol	243.35		NIST Webbook
rinpol	243.76		NIST Webbook
rinpol	240.23		NIST Webbook
rinpol	236.00		NIST Webbook
rinpol	243.30		NIST Webbook
rinpol	240.25		NIST Webbook
rinpol	243.90		NIST Webbook
rinpol	243.10		NIST Webbook
rinpol	240.30		NIST Webbook
rinpol	243.75		NIST Webbook
rinpol	243.56		NIST Webbook
rinpol	243.30		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	240.25		NIST Webbook
rinpol	1415.40		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	243.40		NIST Webbook
rinpol	242.97		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	538.00 ± 4.00	K	NIST Webbook
tb	536.00 ± 8.00	K	NIST Webbook
tb	538.40	K	KDB
tb	538.20	K	Critical properties of some alkylnaphthalenes
tb	536.20	K	NIST Webbook
tb	538.20 ± 0.30	K	NIST Webbook

tc	773.80	K	KDB
tf	269.00	K	KDB
vc	0.521	m3/kmol	KDB
zc	0.2439810		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	0.0012561	Pa×s	309.16	Joback Method
dvisc	0.0008686	Pa×s	345.90	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53563e+01
Coeff. B	-5.33641e+03
Coeff. C	-3.92350e+01
Temperature range (K), min.	393.37
Temperature range (K), max.	570.49

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	7.59707e+01
Coeff. B	-1.02057e+04
Coeff. C	-8.38523e+00
Coeff. D	1.31534e-06
Temperature range (K), min.	283.15
Temperature range (K), max.	585.15

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical properties of some alkylnaphthalenes:	https://www.doi.org/10.1016/j.fluid.2013.08.041
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=771
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C575417&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol771.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

Latest version available from:
https://www.chemeo.com/cid/35-486-4/Naphthalene-1-3-dimethyl.pdf
Generated by Cheméo on 2025-12-05 11:35:52.649080579 +0000 UTC m=+4682750.179121249.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.