Naphthalene, 2-ethyl-

Other names:	.beta.-ethylnaphthalene
	2-Ethylnaphthalene
	BETA-ETHYLNAPHTHALENE
	«beta»-Ethylnaphthalene
	Â«betaÂ»-Ethylnaphthalene
Inchi:	InChI=1S/C12H12/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h3-9H,2H2,1H3
InchiKey:	RJTJVVYSTUQWNI-UHFFFAOYSA-N
Formula:	C12H12
SMILES:	CCc1ccc2ccccc2c1
Mol. weight [g/mol]:	156.22
CAS:	939-27-5

Physical Properties

Property code	Value	Unit	Source
af	0.3920		KDB
ea	0.20 ± 0.06	eV	NIST Webbook
gf	259.59	kJ/mol	Joback Method
hf	125.12	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
ie	7.95	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
log10ws	-4.29		Estimated Solubility Method
log10ws	-4.29		Aqueous Solubility Prediction Method
logp	3.402		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3140.00	kPa	KDB
rinpol	1384.90		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1357.00		NIST Webbook

rinpol	1379.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1343.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1398.10	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1397.00	NIST Webbook
rinpol	1366.00	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1389.60	NIST Webbook
rinpol	1380.60	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1396.10	NIST Webbook
rinpol	1413.70	NIST Webbook
rinpol	1373.30	NIST Webbook
rinpol	1380.60	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1396.10	NIST Webbook
rinpol	1390.60	NIST Webbook
rinpol	1389.60	NIST Webbook
rinpol	1398.00	NIST Webbook
rinpol	1366.00	NIST Webbook
rinpol	1390.00	NIST Webbook
rinpol	1385.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	1378.00	NIST Webbook
rinpol	1385.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1398.00	NIST Webbook
rinpol	1397.30	NIST Webbook
rinpol	1376.00	NIST Webbook
rinpol	1377.00	NIST Webbook
rinpol	238.70	NIST Webbook
rinpol	236.08	NIST Webbook
rinpol	239.06	NIST Webbook
rinpol	238.62	NIST Webbook
rinpol	238.61	NIST Webbook
rinpol	234.68	NIST Webbook
rinpol	237.70	NIST Webbook
rinpol	238.99	NIST Webbook
rinpol	238.50	NIST Webbook
rinpol	239.45	NIST Webbook
rinpol	239.27	NIST Webbook
rinpol	238.55	NIST Webbook

rinpol	236.08		NIST Webbook
rinpol	239.40		NIST Webbook
rinpol	238.50		NIST Webbook
rinpol	233.44		NIST Webbook
rinpol	236.30		NIST Webbook
rinpol	236.10		NIST Webbook
rinpol	239.32		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	237.74		NIST Webbook
rinpol	238.90		NIST Webbook
rinpol	238.50		NIST Webbook
rinpol	239.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1363.70		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	234.56		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1961.00		NIST Webbook
tb	527.20	K	Critical properties of some alkylnaphthalenes
tb	531.50	K	KDB
tc	774.90	K	KDB
tf	265.70 ± 2.00	K	NIST Webbook
tf	266.00	K	KDB
tf	265.75	K	Aqueous Solubility Prediction Method
tf	265.80 ± 1.00	K	NIST Webbook
tf	308.00 ± 3.00	K	NIST Webbook
vc	0.521	m3/kmol	KDB
zc	0.2541570		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.61	J/mol×K	562.99	Joback Method
cpg	325.77	J/mol×K	601.39	Joback Method
cpg	338.92	J/mol×K	639.78	Joback Method
cpg	372.97	J/mol×K	754.97	Joback Method

cpg	351.12	J/mol×K	678.18	Joback Method
cpg	362.44	J/mol×K	716.57	Joback Method
cpg	296.36	J/mol×K	524.60	Joback Method
dvisc	0.0003581	Pa×s	486.61	Joback Method
dvisc	0.0004355	Pa×s	448.61	Joback Method
dvisc	0.0005492	Pa×s	410.62	Joback Method
dvisc	0.0007262	Pa×s	372.63	Joback Method
dvisc	0.0010231	Pa×s	334.63	Joback Method
dvisc	0.0003029	Pa×s	524.60	Joback Method
dvisc	0.0015737	Pa×s	296.64	Joback Method
hvapt	56.70	kJ/mol	479.00	NIST Webbook
hvapt	61.90	kJ/mol	302.50	NIST Webbook
hvapt	64.70	kJ/mol	398.00	NIST Webbook
hvapt	48.12	kJ/mol	531.50	KDB
hvapt	69.30	kJ/mol	333.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48904e+01
Coeff. B	-4.63090e+03
Coeff. C	-7.61770e+01
Temperature range (K), min.	393.30
Temperature range (K), max.	559.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.08322e+02
Coeff. B	-1.14630e+04
Coeff. C	-1.33361e+01
Coeff. D	5.59028e-06
Temperature range (K), min.	391.15
Temperature range (K), max.	566.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C939275&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol769.mol
Critical properties of some alkylnaphthalenes:	https://www.doi.org/10.1016/j.fluid.2013.08.041
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=769

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
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