Naphthalene, 1-ethyl-

Other names:	1-Ethylnaphthalene
	ALPHA-ETHYLNAPHTHALENE
	«alpha»-Ethylnaphthalene
	Â«alphaÂ»-Ethylnaphthalene
Inchi:	InChI=1S/C12H12/c1-2-10-7-5-8-11-6-3-4-9-12(10)11/h3-9H,2H2,1H3
InchiKey:	ZMXIYERNXPIYFR-UHFFFAOYSA-N
Formula:	C12H12
SMILES:	CCc1cccc2ccccc12
Mol. weight [g/mol]:	156.22
CAS:	1127-76-0

Physical Properties

Property code	Value	Unit	Source
af	0.3950		KDB
chl	-6171.00	kJ/mol	NIST Webbook
ea	0.15 ± 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
log10ws	-4.17		Estimated Solubility Method
log10ws	-4.17		Aqueous Solubility Prediction Method
logp	3.402		Crippen Method
mcvol	136.720	ml/mol	McGowan Method
pc	3140.00	kPa	KDB
rinpol	1383.60		NIST Webbook
rinpol	239.92		NIST Webbook
rinpol	236.08		NIST Webbook
rinpol	239.20		NIST Webbook
rinpol	239.70		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1379.00		NIST Webbook

rinpol	1397.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1393.80		NIST Webbook
rinpol	1393.10		NIST Webbook
rinpol	1383.60		NIST Webbook
rinpol	1393.80		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1413.70		NIST Webbook
rinpol	1377.10		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1393.80		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1393.80		NIST Webbook
rinpol	1393.10		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1359.14		NIST Webbook
rinpol	1369.60		NIST Webbook
rinpol	1376.32		NIST Webbook
rinpol	1394.60		NIST Webbook
rinpol	1406.41		NIST Webbook
rinpol	1413.99		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1393.40		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1400.50		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	238.70		NIST Webbook
rinpol	236.56		NIST Webbook
rinpol	239.30		NIST Webbook
rinpol	239.30		NIST Webbook
rinpol	239.24		NIST Webbook
rinpol	237.97		NIST Webbook
rinpol	239.10		NIST Webbook
rinpol	239.72		NIST Webbook
rinpol	239.88		NIST Webbook
rinpol	233.53		NIST Webbook
rinpol	236.56		NIST Webbook
rinpol	240.10		NIST Webbook
rinpol	239.30		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	236.60		NIST Webbook
tb	531.50	K	KDB

tc	774.90	K	KDB
tf	258.00 ± 3.00	K	NIST Webbook
tf	259.27 ± 0.20	K	NIST Webbook
tf	259.25	K	Aqueous Solubility Prediction Method
tf	259.00	K	KDB
vc	0.521	m3/kmol	KDB
zc	0.2541570		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.44	J/mol×K	716.57	Joback Method
cpg	351.12	J/mol×K	678.18	Joback Method
cpg	338.92	J/mol×K	639.78	Joback Method
cpg	325.77	J/mol×K	601.39	Joback Method
cpg	311.61	J/mol×K	562.99	Joback Method
cpg	296.36	J/mol×K	524.60	Joback Method
cpg	372.97	J/mol×K	754.97	Joback Method
dvisc	0.0015737	Pa×s	296.64	Joback Method
dvisc	0.0003029	Pa×s	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
hvapt	48.12	kJ/mol	531.50	KDB
hvapt	57.30	kJ/mol	479.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37996e+01
Coeff. B	-4.28448e+03
Coeff. C	-7.33460e+01
Temperature range (K), min.	390.43

Temperature range (K), max.	578.11

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.07197e+02
Coeff. B	-1.14548e+04
Coeff. C	-1.31370e+01
Coeff. D	4.99842e-06
Temperature range (K), min.	259.34
Temperature range (K), max.	776.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=768

KDB: https://www.cheric.org/files/research/kdb/mol/mol768.mol

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1127760&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

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

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
vc:	Critical Volume
zc:	Critical Compressibility