Naphthalene, 1-chloro-

Other names:	.alpha.-chloronaphthalene
	1-CHLORONAPHTHALENE
	1-Chlornaftalen
	1-Chloronapthalene
	1-NAPHTHYL CHLORIDE
	1-Naphthalenyl chloride
	ALPHA-CHLORONAPHTHALENE
	Monochloro naphthalene
	NSC 6166
	alpha-Naphthyl chloride
	«alpha»-Chlornaphthalene
	«alpha»-Chloronaphthalene
	«alpha»-naphthyl chloride
	Â«alphaÂ»-Chlornaphthalene
	Â«alphaÂ»-Chloronaphthalene
	Â«alphaÂ»-naphthyl chloride
Inchi:	InChI=1S/C10H7Cl/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	JTPNRXUCIXHOKM-UHFFFAOYSA-N
Formula:	C10H7Cl
SMILES:	Clc1cccc2ccccc12
Mol. weight [g/mol]:	162.62
CAS:	90-13-1

Physical Properties

Property code	Value	Unit	Source
chl	-5009.20 ± 8.40	kJ/mol	NIST Webbook
ea	0.28 ± 0.00	eV	NIST Webbook
gf	230.82	kJ/mol	Joback Method
hf	115.00 ± 9.60	kJ/mol	NIST Webbook
hfl	49.80 ± 8.40	kJ/mol	NIST Webbook
hfus	16.52	kJ/mol	Joback Method
hvap	62.00 ± 0.40	kJ/mol	NIST Webbook
hvap	64.00 ± 0.30	kJ/mol	NIST Webbook
hvap	65.30 ± 5.00	kJ/mol	NIST Webbook
hvap	64.70	kJ/mol	NIST Webbook
ie	8.13	eV	NIST Webbook

log10ws	-3.93		Estimated Solubility Method
log10ws	-3.93		Aqueous Solubility Prediction Method
logp	3.493		Crippen Method
mcvol	120.780	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	3655.35	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	236.62		NIST Webbook
rinpol	236.15		NIST Webbook
rinpol	236.90		NIST Webbook
rinpol	1356.10		NIST Webbook
rinpol	1356.10		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook
tb	516.27	K	Joback Method
tc	760.74	K	Joback Method
tf	270.70 ± 0.50	K	NIST Webbook
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.85	J/mol×K	679.25	Joback Method
cpg	258.09	J/mol×K	597.76	Joback Method
cpg	246.83	J/mol×K	557.01	Joback Method
cpg	234.54	J/mol×K	516.27	Joback Method
cpg	286.50	J/mol×K	719.99	Joback Method
cpg	294.46	J/mol×K	760.74	Joback Method
cpg	268.40	J/mol×K	638.50	Joback Method
cpl	211.28	J/mol×K	298.15	NIST Webbook
cpl	212.60	J/mol×K	298.15	NIST Webbook
cpl	211.37	J/mol×K	298.15	NIST Webbook
dvisc	0.0003504	Pa×s	516.27	Joback Method
dvisc	0.0004927	Pa×s	445.52	Joback Method
dvisc	0.0006105	Pa×s	410.14	Joback Method

dvisc	0.0007878	Pa×s	374.77	Joback Method
dvisc	0.0010722	Pa×s	339.39	Joback Method
dvisc	0.0004103	Pa×s	480.89	Joback Method
dvisc	0.0015676	Pa×s	304.02	Joback Method
hfust	12.90	kJ/mol	270.70	NIST Webbook
hfust	12.90	kJ/mol	270.70	NIST Webbook
hvapt	59.60	kJ/mol	453.00	NIST Webbook
hvapt	58.60	kJ/mol	373.00	NIST Webbook
hvapt	57.80	kJ/mol	417.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44380e+01
Coeff. B	-4.44868e+03
Coeff. C	-7.93600e+01
Temperature range (K), min.	393.75
Temperature range (K), max.	566.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.48921e+02
Coeff. B	-1.35878e+04
Coeff. C	-1.93077e+01
Coeff. D	8.49730e-06
Temperature range (K), min.	269.15
Temperature range (K), max.	785.00

Sources

Temperature Dependence of Solubility of Individual Light Fullerenes and Industrial Fullerene Mixture in 1-Chloronaphthalene and 1-Bromonaphthalene:	https://www.doi.org/10.1021/je900814w
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Bromoderivatives C60Brn (n = 6, 8, 24) in 1-Chloronaphthalene and 1-Bromonaphthalene in the Temperature Range (10 to 60) deg C:	https://www.doi.org/10.1021/je100224a
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1710.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90131&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1710
Ternary Liquid-Liquid Equilibria for Systems of (Sulfolane + Toluene or Chloronaphthalene + Octane):	https://www.doi.org/10.1021/je0601210

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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

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