

Naphthalene, 2-chloro-

Other names:	2-Chlornaftalen 2-Chloronaphthalene 2-Chloronaphthalene Chloronaphthalene Rcra waste number U047 «beta»-Chloronaphthalene Â«betaÂ»-Chloronaphthalene
Inchi:	InChI=1S/C10H7Cl/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey:	CGYGETOMCSJHJU-UHFFFAOYSA-N
Formula:	C10H7Cl
SMILES:	Clc1ccc2ccccc2c1
Mol. weight [g/mol]:	162.62
CAS:	91-58-7

Physical Properties

Property code	Value	Unit	Source
chs	-5014.50 ± 8.40	kJ/mol	NIST Webbook
gf	230.82	kJ/mol	Joback Method
hf	137.00 ± 10.00	kJ/mol	NIST Webbook
hfs	55.20 ± 8.40	kJ/mol	NIST Webbook
hfus	16.52	kJ/mol	Joback Method
hsub	82.00 ± 5.90	kJ/mol	NIST Webbook
hvap	62.30 ± 1.10	kJ/mol	NIST Webbook
ie	8.11	eV	NIST Webbook
log10ws	-4.14		Estimated Solubility Method
log10ws	-4.14		Aqueous Solubility Prediction Method
logp	3.493		Crippen Method
mvol	120.780	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1379.00		NIST Webbook
rinpol	235.90		NIST Webbook
rinpol	236.00		NIST Webbook
rinpol	237.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1343.00		NIST Webbook

rinpol	1353.00		NIST Webbook
rinpol	1366.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	1973.00		NIST Webbook
ss	202.13	J/molxK	NIST Webbook
tb	516.27	K	Joback Method
tc	760.74	K	Joback Method
tf	332.00 ± 1.00	K	NIST Webbook
tt	331.17 ± 0.10	K	NIST Webbook
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.54	J/molxK	516.27	Joback Method
cpg	246.83	J/molxK	557.01	Joback Method
cpg	258.09	J/molxK	597.76	Joback Method
cpg	268.40	J/molxK	638.50	Joback Method
cpg	277.85	J/molxK	679.25	Joback Method
cpg	286.50	J/molxK	719.99	Joback Method
cpg	294.46	J/molxK	760.74	Joback Method
cps	235.64	J/molxK	298.15	NIST Webbook
cps	150.00	J/molxK	250.00	NIST Webbook
dvisc	0.0010722	Paxs	339.39	Joback Method
dvisc	0.0015676	Paxs	304.02	Joback Method
dvisc	0.0007878	Paxs	374.77	Joback Method
dvisc	0.0006105	Paxs	410.14	Joback Method
dvisc	0.0004927	Paxs	445.52	Joback Method
dvisc	0.0004103	Paxs	480.89	Joback Method
dvisc	0.0003504	Paxs	516.27	Joback Method
hfust	14.70	kJ/mol	332.00	NIST Webbook
hfust	14.70	kJ/mol	332.00	NIST Webbook
hvapt	57.90	kJ/mol	417.50	NIST Webbook
hvapt	58.50	kJ/mol	373.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33546e+01
Coeff. B	-3.95755e+03
Coeff. C	-8.82540e+01
Temperature range (K), min.	391.12
Temperature range (K), max.	580.30

Sources

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/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91587&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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