

Naphthalene, 1-chloro-2-methyl-

Other names:	1-Chloro-2-methylnaphthalene
Inchi:	InChI=1S/C11H9Cl/c1-8-6-7-9-4-2-3-5-10(9)11(8)12/h2-7H,1H3
InchiKey:	MNCMVFFWMBXFLK-UHFFFAOYSA-N
Formula:	C11H9Cl
SMILES:	Cc1ccc2ccccc2c1Cl
Mol. weight [g/mol]:	176.64
CAS:	5859-45-0

Physical Properties

Property code	Value	Unit	Source
gf	229.61	kJ/mol	Joback Method
hf	118.55	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.802		Crippen Method
mcvol	134.870	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1475.30		NIST Webbook
rinpol	1475.30		NIST Webbook
tb	544.13	K	Joback Method
tc	784.89	K	Joback Method
tf	327.81	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.43	J/molxK	544.13	Joback Method
cpg	290.33	J/molxK	584.26	Joback Method
cpg	302.26	J/molxK	624.38	Joback Method
cpg	313.29	J/molxK	664.51	Joback Method
cpg	323.48	J/molxK	704.64	Joback Method
cpg	332.90	J/molxK	744.77	Joback Method

cpg	341.64	J/mol×K	784.89	Joback Method
dvisc	0.0013413	Paxs	327.81	Joback Method
dvisc	0.0009472	Paxs	363.86	Joback Method
dvisc	0.0007122	Paxs	399.92	Joback Method
dvisc	0.0005614	Paxs	435.97	Joback Method
dvisc	0.0004589	Paxs	472.02	Joback Method
dvisc	0.0003860	Paxs	508.08	Joback Method
dvisc	0.0003322	Paxs	544.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42441e+01
Coeff. B	-4.48838e+03
Coeff. C	-9.81230e+01
Temperature range (K), min.	419.72
Temperature range (K), max.	600.59

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5859450&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/ci9903071

Legend

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
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

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