1-Naphthalenecarbonyl chloride

Other names:	1-Naphthoyl chloride
	«alpha»-Naphthoyl chloride
	1-(Chlorocarbonyl)naphthalene
	1-Naphthoic acid chloride
Inchi:	InChI=1S/C11H7ClO/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	NSNPSJGHTQIXDO-UHFFFAOYSA-N
Formula:	C11H7ClO
SMILES:	O=C(Cl)c1cccc2ccccc12
Mol. weight [g/mol]:	190.63
CAS:	879-18-5

Physical Properties

Property code	Value	Unit	Source
gf	110.32	kJ/mol	Joback Method
hf	17.44	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.219		Crippen Method
mcvol	136.440	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	570.70	K	NIST Webbook
tc	840.63	K	Joback Method
tf	365.22	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.06	J/mol×K	593.02	Joback Method
cpg	302.69	J/mol×K	634.29	Joback Method
cpg	313.33	J/mol×K	675.56	Joback Method
cpg	323.04	J/mol×K	716.82	Joback Method
cpg	331.93	J/mol×K	758.09	Joback Method

cpg	340.07	J/mol×K	799.36	Joback Method
cpg	347.55	J/mol×K	840.63	Joback Method
dvisc	0.0017854	Pa×s	365.22	Joback Method
dvisc	0.0012291	Pa×s	403.19	Joback Method
dvisc	0.0009022	Pa×s	441.15	Joback Method
dvisc	0.0006955	Pa×s	479.12	Joback Method
dvisc	0.0005571	Pa×s	517.09	Joback Method
dvisc	0.0004600	Pa×s	555.05	Joback Method
dvisc	0.0003892	Pa×s	593.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.20	K	4.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C879185&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume