Naphthalene, 1-(chloromethyl)-

Other names:	1-(Chlormethyl)naftalen
	1-(Chloromethyl)naphthalene
	1-Menaphthyl chloride
	1-Naphthylmethyl chloride
	NSC 8473
	Naphthalene, «alpha»-(chloromethyl)-
	Naphthalene, Â«alphaÂ»-(chloromethyl)-
	«alpha»-(Chloromethyl)naphthalene
	«alpha»-Naphthylmethyl chloride
	Â«alphaÂ»-(Chloromethyl)naphthalene
	Â«alphaÂ»-Naphthylmethyl chloride
Inchi:	InChI=1S/C11H9Cl/c12-8-10-6-3-5-9-4-1-2-7-11(9)10/h1-7H,8H2
InchiKey:	XMWGTKZEDLCVIG-UHFFFAOYSA-N
Formula:	C11H9Cl
SMILES:	ClCc1cccc2ccccc12
Mol. weight [g/mol]:	176.64
CAS:	86-52-2

Physical Properties

Property code	Value	Unit	Source
gf	239.24	kJ/mol	Joback Method
hf	130.02	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	49.04	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.579		Crippen Method
mcvol	134.870	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	266.23		NIST Webbook
rinpol	266.23		NIST Webbook
tb	564.70	K	NIST Webbook
tc	778.74	K	Joback Method
tf	315.29	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.47	J/mol×K	778.74	Joback Method
cpg	334.64	J/mol×K	738.81	Joback Method
cpg	325.09	J/mol×K	698.88	Joback Method
cpg	314.72	J/mol×K	658.94	Joback Method
cpg	303.46	J/mol×K	619.01	Joback Method
cpg	291.23	J/mol×K	579.08	Joback Method
cpg	277.94	J/mol×K	539.15	Joback Method
dvisc	0.0016514	Pa×s	315.29	Joback Method
dvisc	0.0003391	Pa×s	539.15	Joback Method
dvisc	0.0004002	Pa×s	501.84	Joback Method
dvisc	0.0004852	Pa×s	464.53	Joback Method
dvisc	0.0006082	Pa×s	427.22	Joback Method
dvisc	0.0007961	Pa×s	389.91	Joback Method
dvisc	0.0011032	Pa×s	352.60	Joback Method
hvapt	59.80	kJ/mol	494.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.20	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42056e+01
Coeff. B	-4.47322e+03
Coeff. C	-9.81230e+01
Temperature range (K), min.	419.52
Temperature range (K), max.	601.06

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86522&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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