

Carbamic chloride, diphenyl-

Other names:	Carbamoyl chloride, diphenyl- Diphenylcarbamoyl chloride Diphenylcarbamyl chloride N,N-Diphenylcarbamoyl chloride
Inchi:	InChI=1S/C13H10ClNO/c14-13(16)15(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H
InchiKey:	XNBKKRFABABBPM-UHFFFAOYSA-N
Formula:	C13H10ClNO
SMILES:	O=C(Cl)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	231.68
CAS:	83-01-2

Physical Properties

Property code	Value	Unit	Source
gf	253.33	kJ/mol	Joback Method
hf	100.62	kJ/mol	Joback Method
hfus	26.33	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.184		Crippen Method
mcvol	170.300	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	653.94	K	Joback Method
tc	904.65	K	Joback Method
tf	401.43	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.92	J/mol×K	653.94	Joback Method
cpg	418.11	J/mol×K	695.73	Joback Method
cpg	430.99	J/mol×K	737.51	Joback Method
cpg	442.66	J/mol×K	779.30	Joback Method
cpg	453.22	J/mol×K	821.08	Joback Method

cpg	462.77	J/mol×K	862.87	Joback Method
cpg	471.42	J/mol×K	904.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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