Phenyl isocyanide dichloride

Inchi: InChI=1S/C7H5Cl2N/c8-7(9)10-6-4-2-1-3-5-6/h1-5H
InchiKey: TTWWZVGVBRPHLE-UHFFFAOYSA-N
Formula: C7H5Cl2N
SMILES: ClC(Cl)=Nc1ccccc1
Mol. weight [g/mol]: 174.03
CAS: 622-44-6

Physical Properties

Property code	Value	Unit	Source
hf	135.26	kJ/mol	Cheméo Relay (1.0)
hvap	50.98	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-2.98		Cheméo Relay (1.0)
logp	3.152		Crippen Method
mcvol	115.890	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	479.69	K	Cheméo Relay (1.0)
tc	706.56	K	Cheméo Relay (1.0)
tf	247.40	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27423e+01
Coeff. B	-4.55099e+03
Temperature range (K), min.	365.40
Temperature range (K), max.	612.45

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point