

2-(2-CHLOROBENZOYL)-PYRIDINE

Other names:	2-(2-Chlorobenzoyl)-pyridine
Inchi:	InChI=1S/C12H8ClNO/c13-10-6-2-1-5-9(10)12(15)11-7-3-4-8-14-11/h1-8H
InchiKey:	XSPNJXJVXUZKPE-UHFFFAOYSA-N
Formula:	C12H8ClNO
SMILES:	O=C(c1ccccc1)c1cccc1Cl
Mol. weight [g/mol]:	217.66

Physical Properties

Property code	Value	Unit	Source
hf	53.42	kJ/mol	Cheméo Relay (1.0)
hvap	88.13	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	NIST Webbook
log10ws	-2.99		Cheméo Relay (1.0)
logp	2.966		Crippen Method
mcvol	156.210	ml/mol	McGowan Method
tb	601.78	K	Cheméo Relay (1.0)
tf	347.36	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1694571&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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