

P-phenylazobenzoyl chloride

Other names:	4-phenylazobenzoyl chloride
Inchi:	InChI=1S/C13H9ClN2O/c14-13(17)10-6-8-12(9-7-10)16-15-11-4-2-1-3-5-11/h1-9H/b16-1
InchiKey:	RYMHZBAYPLCCAC-FOCLMDBBSA-N
Formula:	C13H9ClN2O
SMILES:	O=C(Cl)c1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]:	244.68
CAS:	104-24-5

Physical Properties

Property code	Value	Unit	Source
hf	68.84	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.481		Crippen Method
mcvol	175.980	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
tb	795.68	K	Joback Method
tc	1066.75	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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

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