

4-Isocyanatoacetophenone

Other names:	4-Acetylphenyl isocyanate
Inchi:	InChI=1S/C9H7NO2/c1-7(12)8-2-4-9(5-3-8)10-6-11/h2-5H,1H3
InchiKey:	MOZSVHZOUDIZMF-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	CC(=O)c1ccc(N=C=O)cc1
Mol. weight [g/mol]:	161.16
CAS:	49647-20-3

Physical Properties

Property code	Value	Unit	Source
hf	-122.02	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	1.856		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	557.52	K	Joback Method
tc	785.09	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49647203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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