

2-Carbomethoxyphenyl isocyanate

Other names:	2-Methoxycarbonylphenyl isocyanate
Inchi:	InChI=1S/C9H7NO3/c1-13-9(12)7-4-2-3-5-8(7)10-6-11/h2-5H,1H3
InchiKey:	ATFKBWNEVZUSKC-UHFFFAOYSA-N
Formula:	C9H7NO3
SMILES:	<chem>COC(=O)c1ccccc1N=C=O</chem>
Mol. weight [g/mol]:	177.16
CAS:	1793-07-3

Physical Properties

Property code	Value	Unit	Source
hf	-254.24	kJ/mol	Joback Method
hvap	57.25	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	1.440		Crippen Method
mcvol	128.600	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	579.94	K	Joback Method
tc	804.54	K	Joback Method

Sources

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=C1793073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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