

1-ISOQUINOLINECARBOXYLIC ACID

Other names:	isoquinoline-1-carboxylic acid
Inchi:	InChI=1S/C10H7NO2/c12-10(13)9-8-4-2-1-3-7(8)5-6-11-9/h1-6H,(H,12,13)
InchiKey:	XAAKCCMYRKZRAK-UHFFFAOYSA-N
Formula:	C10H7NO2
SMILES:	O=C(O)c1nccc2ccccc12
Mol. weight [g/mol]:	173.17

Physical Properties

Property code	Value	Unit	Source
hf	-178.73	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-2.18		Cheméo Relay (1.0)
logp	1.933		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
tb	606.32	K	Cheméo Relay (1.0)
tf	425.73	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C486737&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

Legend

hf: Enthalpy of formation 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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<https://www.chemeo.com/cid/83-444-7/1-ISOQUINOLINECARBOXYLIC-ACID.pdf>

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