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