

1(2H)-Quinolinecarboxylic acid, 2-cyano-, ethyl ester

Other names:	2-Cyano-1(2H)-quinolinecarboxylic acid, ethyl ester
Inchi:	InChI=1S/C13H12N2O2/c1-2-17-13(16)15-11(9-14)8-7-10-5-3-4-6-12(10)15/h3-8,11H,2H
InchiKey:	QFAHEDSFVHOFGW-UHFFFAOYSA-N
Formula:	C13H12N2O2
SMILES:	CCOC(=O)N1c2ccccc2C=CC1C#N
Mol. weight [g/mol]:	228.25
CAS:	17954-23-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	2.568		Crippen Method
mcvol	173.910	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.88	kJ/mol	337.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17954233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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