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/ci990307l
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