Coumarin, 3-thiocyano-4-methyl-7-(N,N-diethylamino)-

Inchi: InChI=1S/C15H16N2O2S/c1-4-17(5-2)11-6-7-12-10(3)14(20-9-16)15(18)19-13(12)8-11/h

InchiKey: KGDNJUMHXJGLRF-UHFFFAOYSA-N

Formula: C15H16N2O2S

SMILES: CCN(CC)c1ccc2c(C)c(SC#N)c(=O)oc2c1

Mol. weight [g/mol]: 288.37

CAS: 114171-77-6

Physical Properties

Property code	Value	Unit	Source
ie	7.75	eV	NIST Webbook
log10ws	-8.76		Crippen Method
logp	3.521		Crippen Method
mcvol	218.440	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C114171776&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.