2H-1-Benzopyran-2-one, 7-(diethylamino)-4-(trifluoromethyl)-

Other names: 7-(Diethylamino)-4-(trifluoromethyl)-2H-1-benzopyran-2-one
7-(diethylamino)-4-(trifluoromethyl)-2-benzopyrone
4-Trifluoromethyl-7-(N,N-diethylamino)coumarin

Inchi: InChI=1S/C14H14F3NO2/c1-3-18(4-2)9-5-6-10-11(14(15,16)17)8-13(19)20-12(10)7-9/h5

InchiKey: UIMOXRDVWDLOHW-UHFFFAOYSA-N

Formula: C14H14F3NO2

SMILES: CCN(CC)c1ccc2c(C(F)(F)F)cc(=O)oc2c1

Mol. weight [g/mol]: 285.26

CAS: 41934-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	3.658		Crippen Method
mcvol	191.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.30	kJ/mol	360.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41934478&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

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