

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

<b>Other names:</b>	7-(Diethylamino)-4-(trifluoromethyl)-2H-1-benzopyran-2-one 7-(diethylamino)-4-(trifluoromethyl)-2-benzopyrone 4-Trifluoromethyl-7-(N,N-diethylamino)coumarin
<b>Inchi:</b>	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
<b>InchiKey:</b>	UIMOXRDVWDLOHW-UHFFFAOYSA-N
<b>Formula:</b>	C14H14F3NO2
<b>SMILES:</b>	CCN(CC)c1ccc2c(C(F)(F)F)cc(=O)oc2c1
<b>Mol. weight [g/mol]:</b>	285.26
<b>CAS:</b>	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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C41934478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41934478&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

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

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