

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

Other names:	7-Amino-4-(trifluoromethyl)coumarin Coumarin 151 7-Amino-4-trifluoromethyl-chromen-2-one 7-amino-4-(trifluoromethyl)-2-benzopyrone 4-Trifluoromethyl-7-aminocoumarin
Inchi:	InChI=1S/C10H6F3NO2/c11-10(12,13)7-4-9(15)16-8-3-5(14)1-2-6(7)8/h1-4H,14H2
InchiKey:	JBNOVHJXQSHGRL-UHFFFAOYSA-N
Formula:	C10H6F3NO2
SMILES:	<chem>Nc1ccc2c(C(F)(F)F)cc(=O)oc2c1</chem>
Mol. weight [g/mol]:	229.16
CAS:	53518-15-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.17		Crippen Method
logp	2.394		Crippen Method
mcpvol	135.570	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	31.70	kJ/mol	494.80	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53518153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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