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: Nc1ccc2c(C(F)(F)F)cc(=O)oc2c1

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
mcvol	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/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