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

Other names: 4-Methyl-7-(diethylamino)coumarin
7-(Diethylamino)-4-methyl-2H-1-benzopyran-2-one
7-(Diethylamino)-4-methylcoumarin
7-(diethylamino)-4-methyl-2-benzopyrone
7-diethylamino-4-methylchromen-2-one
7D4MC
Aclarat 8678
Blancophor AW
Blancophor FFG
C 47
Calcofluor White RW
Calcofluor White SD
Coumarin 1
Coumarin 460
Coumarin 47
Coumarin, 7-(diethylamino)-4-methyl-
Hakkol P
MDAC
NSC 61830
Uvitex WGS

Inchi: InChI=1S/C14H17NO2/c1-4-15(5-2)11-6-7-12-10(3)8-14(16)17-13(12)9-11/h6-9H,4-5H2,

InchiKey: AFYCEAFSNDLKSX-UHFFFAOYSA-N

Formula: C14H17NO2

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

Mol. weight [g/mol]: 231.29

CAS: 91-44-1

Physical Properties

Property code	Value	Unit	Source
ie	7.38	eV	NIST Webbook
log10ws	-4.00		Aqueous Solubility Prediction Method
logp	2.948		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
tf	344.39 ± 0.30	K	NIST Webbook
tf	344.85 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.88	kJ/mol	343.80	NIST Webbook
sfust	46.26	J/mol×K	343.80	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91441&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point

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