Coumarine, 7-diethylamino-

Other names: Coumarine, 7-diethylamino-
Coumarin, 7-diethylamino-
7-(diethylamino)-2-benzopyrone
Inchi: InChI=1S/C13H15NO2/c1-3-14(4-2)11-7-5-10-6-8-13(15)16-12(10)9-11/h5-9H,3-4H2,1-2
InchiKey: QXAMGWKESXGGNV-UHFFFAOYSA-N
Formula: C13H15NO2
SMILES: CCN(CC)c1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]: 217.27

Physical Properties

Property code	Value	Unit	Source
hf	-221.16	kJ/mol	Cheméo Relay (1.0)
ie	7.41	eV	NIST Webbook
log10ws	-3.63		Cheméo Relay (1.0)
logp	2.639		Crippen Method
mcvol	172.530	ml/mol	McGowan Method
tb	641.94	K	Cheméo Relay (1.0)
tf	391.61	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20571420&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point