6-AMINOCOUMARIN

Other names: Coumarin, 6-amino-
6-Amino-1,2-benzopyrone
6-Aminocoumarin
Inchi: InChI=1S/C9H7NO2/c10-7-2-3-8-6(5-7)1-4-9(11)12-8/h1-5H,10H2
InchiKey: ZOJAINJCZSVZGW-UHFFFAOYSA-N
Formula: C9H7NO2
SMILES: Nc1ccc2oc(=O)ccc2c1
Mol. weight [g/mol]: 161.16

Physical Properties

Property code	Value	Unit	Source
hf	-171.17	kJ/mol	Cheméo Relay (1.0)
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	1.375		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	636.95	K	Cheméo Relay (1.0)
tf	435.55	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14415442&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
Cheméo Relay (1.0):

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point