3-METHYLCOUMARIN

Other names:	Coumarin, 3-methyl-
	3-Methylcoumarin
	3-Methylcumarin
	3-Methyl-2H-1-benzopyran-2-one
Inchi:	InChI=1S/C10H8O2/c1-7-6-8-4-2-3-5-9(8)12-10(7)11/h2-6H,1H3
InchiKey:	VIIIJFZJKFXOGG-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	Cc1cc2ccccc2oc1=O
Mol. weight [g/mol]:	160.17

Physical Properties

Property code	Value	Unit	Source
af	0.4683		Cheméo Relay (1.0)
hf	-195.24	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-2.37		Cheméo Relay (1.0)
logp	2.101		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
pc	4069.85	kPa	Cheméo Relay (1.0, beta)
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
tb	565.70	K	NIST Webbook
tc	798.12	K	Cheméo Relay (1.0)
tf	338.90	K	Cheméo Relay (1.0)
vc	0.453	m3/kmol	Cheméo Relay (1.0)

Sources

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):	

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445821&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume