4(3H)-quinazolinone, 2,3-dimethyl-

Other names:	2,3-Dimethyl-4(3H)-quinazolinone
	Dimethylquinazolone
	Quinazolin-4(3H)-one, 2,3-dimethyl-
	4-Quinazolone, 2,3-dimethyl
	Quinazolin-4-one, 2,3-dimethyl
Inchi:	InChI=1S/C10H10N2O/c1-7-11-9-6-4-3-5-8(9)10(13)12(7)2/h3-6H,1-2H3
InchiKey:	DCKUAHKIBNUXHX-UHFFFAOYSA-N
Formula:	C10H10N2O
SMILES:	Cc1nc2ccccc2c(=O)n1C
Mol. weight [g/mol]:	174.20

Physical Properties

Property code	Value	Unit	Source
af	0.5118		Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-1.07		Cheméo Relay (1.0)
logp	1.242		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	3817.63	kPa	Cheméo Relay (1.0, beta)
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
tb	592.73	K	Cheméo Relay (1.0)
tc	847.85	K	Cheméo Relay (1.0)
tf	432.41	K	Cheméo Relay (1.0)

Sources

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=C1769251&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point