

Quinazolin-4-one, 3-ethyl

Other names:	4-Quinazolone, 3-ethyl
Inchi:	InChI=1S/C10H10N2O/c1-2-12-7-11-9-6-4-3-5-8(9)10(12)13/h3-7H,2H2,1H3
InchiKey:	BMFONNKQZRYQSO-UHFFFAOYSA-N
Formula:	C10H10N2O
SMILES:	CCn1cnc2ccccc2c1=O
Mol. weight [g/mol]:	174.20
CAS:	3476-65-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.416		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3476651&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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