QUINETHAZONE

Other names:	2-Ethyl-7-chloro-1,2,3,4-tetrahydro-4-oxoquinazoline-6-sulfonamide
	6-Quinazolinesulfonamide, 7-chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-
	7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinazolinesulfonamide
	7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinzaolinesulfonamide
	7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-sulfamoylquinazoline
	7-Chloro-2-ethyl-6-sulfamoyl-1,2,3,4-tetrahydro-4-quinazolinone
	7-chloro-2-ethyl-4-oxo-2,3-dihydro-1H-quinazoline-6-sulfonamide
	Aquamox
	CL 36010
	Chinetazone
	Hydromox
	Idrokin
	Quinethazon
	Quinethazone Me
	Quinethazonum
Inchi:	InChI=1S/C10H12ClN3O3S/c1-2-9-13-7-4-6(11)8(18(12,16)17)3-5(7)10(15)14-9/h3-4,9,1
InchiKey:	AGMMTXLNIQSRCG-UHFFFAOYSA-N
Formula:	C10H12ClN3O3S
SMILES:	CCC1NC(=O)c2cc(S(N)(=O)=O)c(Cl)cc2N1
Mol. weight [g/mol]:	289.74

Physical Properties

Property code	Value	Unit	Source
hfus	50.03	kJ/mol	Joback Method
log10ws	-3.29		Aqueous Solubility Prediction Method
log10ws	-3.29		Estimated Solubility Method
logp	0.879		Crippen Method
mcvol	188.980	ml/mol	McGowan Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tf	511.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.68	J/mol×K	803.49	Joback Method
cpg	530.98	J/mol×K	845.30	Joback Method
cpg	541.90	J/mol×K	887.12	Joback Method
cpg	551.40	J/mol×K	928.93	Joback Method
cpg	559.43	J/mol×K	970.75	Joback Method
cpg	565.95	J/mol×K	1012.56	Joback Method
cpg	570.93	J/mol×K	1054.38	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73494&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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