

7-Chloroquinaldine

Other names:	7-Chloro-2-methyl-quinoline 7-chloro-2-methylquinoline
Inchi:	InChI=1S/C10H8ClN/c1-7-2-3-8-4-5-9(11)6-10(8)12-7/h2-6H,1H3
InchiKey:	WQZQFYRSYLXBGP-UHFFFAOYSA-N
Formula:	C10H8ClN
SMILES:	Cc1ccc2ccc(Cl)cc2n1
Mol. weight [g/mol]:	177.63

Physical Properties

Property code	Value	Unit	Source
af	0.4179		Cheméo Relay (1.0)
hf	112.62	kJ/mol	Cheméo Relay (1.0)
hvap	70.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.70		Cheméo Relay (1.0)
logp	3.197		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
pc	4070.01	kPa	Cheméo Relay (1.0, beta)
tb	550.03	K	Cheméo Relay (1.0)
tc	815.94	K	Cheméo Relay (1.0)
tf	346.12	K	Research on the application of 7-chloro-quinaldine adducts in 7-chloro-quinaldine separation process

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	0.07	NIST Webbook

Sources

Research on the application of
7-chloro-quinaldine adducts in
NIST Webbook
7-chloro-quinaldine separation
process:
McGowan Method:

<https://www.doi.org/10.1016/j.jct.2019.02.002>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4965337&Units=SI>

<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):

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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