1,4-Naphthalenedione, 2-amino-3-chloro-

Other names:	Quinoclamine
	ACN
	ACNQ
	2-Amino-3-chloronaphthoquinone
	2-Amino-3-chloro-1,4-naphthoquinone
	2-Chloro-3-amino-1,4-naphthoquinone
	3-Chloro-2-amino-1,4-naphthoquinone
	Mogeton
	1,4-Naphthoquinone, 2-amino-3-chloro-
	06K-Quinone
	O 6K-quinone
	Mogeton G
	Mogeton granule
	06K
	06K-50W
	NSC 3910
	NSC 642009
	Quinoclamin
Inchi:	InChI=1S/C10H6ClNO2/c11-7-8(12)10(14)6-4-2-1-3-5(6)9(7)13/h1-4H,12H2
InchiKey:	OBLNWSCLAYSJJR-UHFFFAOYSA-N
Formula:	C10H6ClNO2
SMILES:	NC1=C(Cl)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	207.61
CAS:	2797-51-5

Physical Properties

Property code	Value	Unit	Source
gf	12.50	kJ/mol	Joback Method
hf	-160.20	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.475		Crippen Method
mcvol	138.200	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1968.00		NIST Webbook

rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	730.26	K	Joback Method
tc	1005.50	K	Joback Method
tf	535.48	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.29	J/mol×K	730.26	Joback Method
cpg	353.66	J/mol×K	776.13	Joback Method
cpg	363.99	J/mol×K	822.01	Joback Method
cpg	373.24	J/mol×K	867.88	Joback Method
cpg	381.39	J/mol×K	913.75	Joback Method
cpg	388.42	J/mol×K	959.63	Joback Method
cpg	394.29	J/mol×K	1005.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2797515&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume