Anthraquinone, 2-amino-3-chloro-

Other names: 2-Amino-3-chloroanthraquinone
3-x-2-AA
Anthraquinone, 2-amino-3-chloro-
Inchi: InChI=1S/C14H8ClNO2/c15-11-5-9-10(6-12(11)16)14(18)8-4-2-1-3-7(8)13(9)17/h1-6H,16
InchiKey: VMOJFUJVEWWUAV-UHFFFAOYSA-N
Formula: C14H8ClNO2
SMILES: Nc1cc2c(cc1Cl)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 257.68

Physical Properties

Property code	Value	Unit	Source
hf	-120.54	kJ/mol	Cheméo Relay (1.0)
hfus	26.12	kJ/mol	Joback Method
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-4.76		Cheméo Relay (1.0)
logp	2.698		Crippen Method
mcvol	175.100	ml/mol	McGowan Method
tb	676.10	K	Cheméo Relay (1.0)
tf	480.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.37	J/mol×K	845.74	Joback Method
cpg	484.65	J/mol×K	892.39	Joback Method
cpg	494.74	J/mol×K	939.05	Joback Method
cpg	503.68	J/mol×K	985.70	Joback Method
cpg	511.49	J/mol×K	1032.36	Joback Method
cpg	518.22	J/mol×K	1079.01	Joback Method
cpg	523.89	J/mol×K	1125.67	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84468&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point