9,10-Anthracenedione, 2-chloro-

Other names:	Anthraquinone, 2-chloro-
	«beta»-Chloroanthraquinone
	2-Chloro-9,10-anthraquinone
	2-Chloroanthraquinone
	2-Chloro-9,10-anthracenedione
Inchi:	InChI=1S/C14H7ClO2/c15-8-5-6-11-12(7-8)14(17)10-4-2-1-3-9(10)13(11)16/h1-7H
InchiKey:	FPKCTSIVDAWGFA-UHFFFAOYSA-N
Formula:	C14H7ClO2
SMILES:	O=C1c2ccccc2C(=O)c2cc(Cl)ccc21
Mol. weight [g/mol]:	242.66
CAS:	131-09-9

Physical Properties

Property code	Value	Unit	Source
gf	86.38	kJ/mol	Joback Method
hf	-85.48	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.115		Crippen Method
mcvol	165.120	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	355.88		NIST Webbook
rinpol	356.47		NIST Webbook
rinpol	353.00		NIST Webbook
rinpol	356.00		NIST Webbook
tb	768.23	K	Joback Method
tc	1045.44	K	Joback Method
tf	482.95 ± 0.20	K	NIST Webbook
tf	482.85 ± 0.30	K	NIST Webbook
tf	483.55 ± 0.40	K	NIST Webbook
tf	483.15 ± 1.00	K	NIST Webbook
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.60	J/mol×K	768.23	Joback Method
cpg	434.19	J/mol×K	814.43	Joback Method
cpg	445.60	J/mol×K	860.63	Joback Method
cpg	455.86	J/mol×K	906.84	Joback Method
cpg	465.03	J/mol×K	953.04	Joback Method
cpg	473.13	J/mol×K	999.24	Joback Method
cpg	480.23	J/mol×K	1045.44	Joback Method
hfust	38.96	kJ/mol	483.02	NIST Webbook
hfust	39.00	kJ/mol	483.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C131099&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
hfust:	Enthalpy of fusion at a given temperature
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

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