Anthracene, 2-chloro-

Other names:	2-Chloroanthracene
	«beta»-Chloro anthracene
	Â«betaÂ»-Chloro anthracene
Inchi:	InChI=1S/C14H9Cl/c15-14-6-5-12-7-10-3-1-2-4-11(10)8-13(12)9-14/h1-9H
InchiKey:	OWFINXQLBMJDJQ-UHFFFAOYSA-N
Formula:	C14H9Cl
SMILES:	Clc1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]:	212.67
CAS:	17135-78-3

Physical Properties

Property code	Value	Unit	Source
ea	0.80 ± 0.10	eV	NIST Webbook
gf	361.52	kJ/mol	Joback Method
hf	247.70	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.646		Crippen Method
mcvol	157.680	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	631.75	K	Joback Method
tc	889.70	K	Joback Method
tf	394.32	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.66	J/mol×K	889.70	Joback Method
cpg	370.92	J/mol×K	674.74	Joback Method
cpg	383.03	J/mol×K	717.73	Joback Method
cpg	394.12	J/mol×K	760.72	Joback Method
cpg	404.32	J/mol×K	803.71	Joback Method

cpg	413.79	J/mol×K	846.71	Joback Method
cpg	357.63	J/mol×K	631.75	Joback Method
dvisc	0.0005552	Pa×s	592.18	Joback Method
dvisc	0.0006369	Pa×s	552.61	Joback Method
dvisc	0.0007463	Pa×s	513.04	Joback Method
dvisc	0.0008980	Pa×s	473.46	Joback Method
dvisc	0.0011176	Pa×s	433.89	Joback Method
dvisc	0.0004923	Pa×s	631.75	Joback Method
dvisc	0.0014534	Pa×s	394.32	Joback Method
hsubt	99.30 ± 2.70	kJ/mol	351.00	NIST Webbook
psub	7.29e-05	kPa	351.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.03e-04	kPa	355.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	5.71e-05	kPa	349.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.24e-04	kPa	358.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.35e-04	kPa	358.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	1.79e-04	kPa	361.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	1.95e-04	kPa	363.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	2.17e-04	kPa	363.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	2.84e-04	kPa	367.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	

psub	3.14e-04	kPa	368.10	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	3.55e-04	kPa	370.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	4.00e-04	kPa	371.80	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.70e-05	kPa	343.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	2.40e-05	kPa	341.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	2.08e-05	kPa	338.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	9.70e-06	kPa	333.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	8.30e-06	kPa	331.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	8.76e-05	kPa	352.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.00e-04	kPa	355.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique:	https://www.doi.org/10.1016/j.jct.2007.09.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17135783&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation 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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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