9-Chloroanthracene

Other names: Anthracene, 9-chloro-
Inchi: InChI=1S/C14H9Cl/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H
InchiKey: KULLJOPUZUWTMF-UHFFFAOYSA-N
Formula: C14H9Cl
SMILES: Clc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 212.67
CAS: 716-53-0

Physical Properties

Property code	Value	Unit	Source
ea	0.86 ± 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
ie	7.45 ± 0.03	eV	NIST Webbook
ie	7.45 ± 0.03	eV	NIST Webbook
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	413.79	J/mol×K	846.71	Joback Method
cpg	404.32	J/mol×K	803.71	Joback Method
cpg	394.12	J/mol×K	760.72	Joback Method
cpg	383.03	J/mol×K	717.73	Joback Method

cpg	370.92	J/mol×K	674.74	Joback Method
cpg	357.63	J/mol×K	631.75	Joback Method
dvisc	0.0014534	Pa×s	394.32	Joback Method
dvisc	0.0004923	Pa×s	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
hfust	18.66	kJ/mol	379.20	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C716530&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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume