

Anthracene, 1-chloro-

Other names:	1-Chloroanthracene
Inchi:	InChI=1S/C14H9Cl/c15-14-7-3-6-12-8-10-4-1-2-5-11(10)9-13(12)14/h1-9H
InchiKey:	SRIHSAFSOOUEGL-UHFFFAOYSA-N
Formula:	C14H9Cl
SMILES:	Clc1cccc2cc3ccccc3cc12
Mol. weight [g/mol]:	212.67
CAS:	4985-70-0

Physical Properties

Property code	Value	Unit	Source
ea	0.83 ± 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	357.63	J/molxK	631.75	Joback Method
cpg	370.92	J/molxK	674.74	Joback Method
cpg	383.03	J/molxK	717.73	Joback Method
cpg	394.12	J/molxK	760.72	Joback Method
cpg	404.32	J/molxK	803.71	Joback Method
cpg	413.79	J/molxK	846.71	Joback Method
cpg	422.66	J/molxK	889.70	Joback Method

dvisc	0.0014534	Paxs	394.32	Joback Method
dvisc	0.0011176	Paxs	433.89	Joback Method
dvisc	0.0008980	Paxs	473.46	Joback Method
dvisc	0.0007463	Paxs	513.04	Joback Method
dvisc	0.0006369	Paxs	552.61	Joback Method
dvisc	0.0005552	Paxs	592.18	Joback Method
dvisc	0.0004923	Paxs	631.75	Joback Method
hfust	14.14	kJ/mol	355.20	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=C4985700&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
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

Latest version available from:

<https://www.chemeo.com/cid/33-509-0/Anthracene-1-chloro.pdf>

Generated by Cheméo on 2024-04-30 15:24:13.503740156 +0000 UTC m=+16779902.424317468.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.