

9-Chlorophenanthrene

Other names:	Phenanthrene, 9-chloro- 10-Chlorophenanthrene
Inchi:	InChI=1S/C14H9Cl/c15-14-9-10-5-1-2-6-11(10)12-7-3-4-8-13(12)14/h1-9H
InchiKey:	CJWHZQNUDAJJSB-UHFFFAOYSA-N
Formula:	C14H9Cl
SMILES:	Clc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	212.67
CAS:	947-72-8

Physical Properties

Property code	Value	Unit	Source
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.63	J/mol×K	631.75	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	422.66	J/mol×K	889.70	Joback Method

dvisc	0.0004923	Paxs	631.75	Joback Method
dvisc	0.0005552	Paxs	592.18	Joback Method
dvisc	0.0006369	Paxs	552.61	Joback Method
dvisc	0.0007463	Paxs	513.04	Joback Method
dvisc	0.0008980	Paxs	473.46	Joback Method
dvisc	0.0011176	Paxs	433.89	Joback Method
dvisc	0.0014534	Paxs	394.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C947728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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

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