

Acenaphthene, 1-chloro

Inchi:	InChI=1S/C12H9Cl/c13-11-7-9-5-1-3-8-4-2-6-10(11)12(8)9/h1-6,11H,7H2
InchiKey:	ANIXIYQBGBGRI-UHFFFAOYSA-N
Formula:	C12H9Cl
SMILES:	<chem>C1C1Cc2cccc3cccc1c23</chem>
Mol. weight [g/mol]:	188.65

Physical Properties

Property code	Value	Unit	Source
gf	310.88	kJ/mol	Joback Method
hf	176.87	kJ/mol	Joback Method
hfus	21.55	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.676		Crippen Method
mcvol	138.100	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinsol	1706.00		NIST Webbook
tb	569.48	K	Joback Method
tc	814.84	K	Joback Method
tf	360.54	K	Joback Method
vc	0.535	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.12	J/molxK	569.48	Joback Method
cpg	320.61	J/molxK	610.37	Joback Method
cpg	332.93	J/molxK	651.27	Joback Method
cpg	344.20	J/molxK	692.16	Joback Method
cpg	354.56	J/molxK	733.06	Joback Method
cpg	364.15	J/molxK	773.95	Joback Method
cpg	373.10	J/molxK	814.84	Joback Method
dvisc	0.0015704	Paxs	360.54	Joback Method
dvisc	0.0013845	Paxs	395.36	Joback Method

dvisc	0.0012457	Paxs	430.19	Joback Method
dvisc	0.0011387	Paxs	465.01	Joback Method
dvisc	0.0010541	Paxs	499.83	Joback Method
dvisc	0.0009855	Paxs	534.66	Joback Method
dvisc	0.0009291	Paxs	569.48	Joback Method

Sources

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=R131581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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