1H-Phenalene

Other names:	Phenalene
	Peri-Naphthindene
	Perinaphthene
	1H-Benzonaphthene
Inchi:	InChI=1S/C13H10/c1-4-10-6-2-8-12-9-3-7-11(5-1)13(10)12/h1-8H,9H2
InchiKey:	XDJOIMJURHQYDW-UHFFFAOYSA-N
Formula:	C13H10
SMILES:	C1=Cc2cccc3cccc(c23)C1
Mol. weight [g/mol]:	166.22
CAS:	203-80-5

Physical Properties

Property code	Value	Unit	Source
gf	356.80	kJ/mol	Joback Method
hf	243.93	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.409		Crippen Method
mcvol	135.650	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	268.00		NIST Webbook
rinpol	258.62		NIST Webbook
rinpol	266.80		NIST Webbook
rinpol	267.20		NIST Webbook
rinpol	267.80		NIST Webbook
rinpol	266.90		NIST Webbook
rinpol	268.00		NIST Webbook
tb	563.03	K	Joback Method
tc	810.68	K	Joback Method
tf	343.37	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.80	J/mol×K	563.03	Joback Method
cpg	321.41	J/mol×K	604.30	Joback Method
cpg	334.73	J/mol×K	645.58	Joback Method
cpg	346.90	J/mol×K	686.85	Joback Method
cpg	358.06	J/mol×K	728.13	Joback Method
cpg	368.35	J/mol×K	769.40	Joback Method
cpg	377.92	J/mol×K	810.68	Joback Method
dvisc	0.0014835	Pa×s	343.37	Joback Method
dvisc	0.0011839	Pa×s	379.98	Joback Method
dvisc	0.0009831	Pa×s	416.59	Joback Method
dvisc	0.0008412	Pa×s	453.20	Joback Method
dvisc	0.0007367	Pa×s	489.81	Joback Method
dvisc	0.0006572	Pa×s	526.42	Joback Method
dvisc	0.0005951	Pa×s	563.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C203805&Units=SI

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

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