

1,4-Methanonaphthalene, 1,4-dihydro-

Other names:	Benzenorbornadiene 1,4-Dihydro-1,4-methanonaphthalene
Inchi:	InChI=1S/C11H10/c1-2-4-11-9-6-5-8(7-9)10(11)3-1/h1-6,8-9H,7H2
InchiKey:	IEGYXSAHRKJELM-UHFFFAOYSA-N
Formula:	C11H10
SMILES:	C1=CC2CC1c1cccc12
Mol. weight [g/mol]:	142.20
CAS:	4453-90-1

Physical Properties

Property code	Value	Unit	Source
gf	308.08	kJ/mol	Joback Method
hf	164.23	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	42.96	kJ/mol	Joback Method
ie	8.32 ± 0.05	eV	NIST Webbook
ie	8.34 ± 0.05	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	8.30 ± 0.05	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.827		Crippen Method
mvol	116.070	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	491.11	K	Joback Method
tc	722.56	K	Joback Method
tf	292.83	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.76	J/mol×K	491.11	Joback Method
cpg	322.20	J/mol×K	683.98	Joback Method

cpg	311.12	J/mol×K	645.41	Joback Method
cpg	299.05	J/mol×K	606.83	Joback Method
cpg	285.89	J/mol×K	568.26	Joback Method
cpg	271.50	J/mol×K	529.68	Joback Method
cpg	332.43	J/mol×K	722.56	Joback Method
dvisc	0.0009547	Paxs	491.11	Joback Method
dvisc	0.0009530	Paxs	458.06	Joback Method
dvisc	0.0009509	Paxs	425.02	Joback Method
dvisc	0.0009486	Paxs	391.97	Joback Method
dvisc	0.0009458	Paxs	358.92	Joback Method
dvisc	0.0009425	Paxs	325.88	Joback Method
dvisc	0.0009385	Paxs	292.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4453901&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
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

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