

1,4-Methanonaphthalen-9-ol,1,2,3,4-tetrahydro-6-methoxy-

Inchi:

LnChI=1S/C12H14O/c1-7-2-3-8-9-4-5-10(12(9)13)11(8)6-7/h2-3,6,9-10,12-13H,4-5H2,1H1

InchiKey:

ANPDCXWZMJATJ-UVTZGIPTSA-N

Formula:

C12H14O

SMILES:

Cc1ccc2c(c1)C1CCC2C1O

Mol. weight [g/mol]:

174.24

CAS:

16306-85-7

Physical Properties

Property code	Value	Unit	Source
gf	132.38	kJ/mol	Joback Method
hf	-98.23	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
ie	8.41 ± 0.02	eV	NIST Webbook
log10ws	-3.06		Crippen Method
logp	2.331		Crippen Method
mcvol	140.330	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	607.32	K	Joback Method
tc	816.51	K	Joback Method
tf	372.44	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.41	J/mol×K	607.32	Joback Method
cpg	439.17	J/mol×K	781.65	Joback Method
cpg	428.32	J/mol×K	746.78	Joback Method
cpg	416.81	J/mol×K	711.92	Joback Method
cpg	404.53	J/mol×K	677.05	Joback Method
cpg	391.43	J/mol×K	642.19	Joback Method
cpg	449.42	J/mol×K	816.51	Joback Method
dvisc	0.0006118	Pa×s	607.32	Joback Method

dvisc	0.0007334	Pa×s	568.17	Joback Method
dvisc	0.0009031	Pa×s	529.03	Joback Method
dvisc	0.0011496	Pa×s	489.88	Joback Method
dvisc	0.0015262	Pa×s	450.73	Joback Method
dvisc	0.0021383	Pa×s	411.59	Joback Method
dvisc	0.0032160	Pa×s	372.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16306857&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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