

1-Methyl-1,2,3,4,-tetrahydronaphthalene-1-hydrop

Inchi:	InChI=1S/C11H14O2/c1-11(13-12)8-4-6-9-5-2-3-7-10(9)11/h2-3,5,7,12H,4,6,8H2,1H3
InchiKey:	BEVOTSGQUUDZQKM-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CC1(OO)CCc2ccccc21
Mol. weight [g/mol]:	178.23
CAS:	99964-59-7

Physical Properties

Property code	Value	Unit	Source
chs	-6172.20	kJ/mol	NIST Webbook
gf	-54.14	kJ/mol	Joback Method
hf	-247.88	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.728		Crippen Method
mvol	142.970	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	608.59	K	Joback Method
tc	825.39	K	Joback Method
tf	374.04	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.12	J/molxK	608.59	Joback Method
cpg	380.73	J/molxK	644.72	Joback Method
cpg	393.53	J/molxK	680.86	Joback Method
cpg	405.65	J/molxK	716.99	Joback Method
cpg	417.21	J/molxK	753.12	Joback Method
cpg	428.35	J/molxK	789.25	Joback Method
cpg	439.19	J/molxK	825.39	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=C99964597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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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