1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-, stereoisomer

Other names: 1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetrahydro-, anti-
anti-7-Benzonorbornenol
anti-7-Hydroxybenzonorbornene

Inchi: InChI=1S/C11H12O/c12-11-9-5-6-10(11)8-4-2-1-3-7(8)9/h1-4,9-12H,5-6H2

InchiKey: HEKIGGFOVMNILV-UHFFFAOYSA-N

Formula: C11H12O

SMILES: OC1C2CCC1c1ccccc12

Mol. weight [g/mol]: 160.21

CAS: 1198-20-5

Physical Properties

Property code	Value	Unit	Source
gf	133.59	kJ/mol	Joback Method
hf	-66.12	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
ie	8.62 ± 0.02	eV	NIST Webbook
ie	8.80 ± 0.02	eV	NIST Webbook
log10ws	-2.59		Crippen Method
logp	2.022		Crippen Method
mcvol	126.240	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	579.46	K	Joback Method
tc	791.10	K	Joback Method
tf	348.65	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.80	J/mol×K	579.46	Joback Method
cpg	389.36	J/mol×K	755.83	Joback Method
cpg	379.04	J/mol×K	720.55	Joback Method
cpg	368.02	J/mol×K	685.28	Joback Method

cpg	356.20	J/mol×K	650.01	Joback Method
cpg	343.49	J/mol×K	614.73	Joback Method
cpg	399.04	J/mol×K	791.10	Joback Method
dvisc	0.0006585	Pa×s	579.46	Joback Method
dvisc	0.0007969	Pa×s	540.99	Joback Method
dvisc	0.0009931	Pa×s	502.52	Joback Method
dvisc	0.0012835	Pa×s	464.06	Joback Method
dvisc	0.0017377	Pa×s	425.59	Joback Method
dvisc	0.0024985	Pa×s	387.12	Joback Method
dvisc	0.0038921	Pa×s	348.65	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1198205&Units=SI

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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