

1,4:5,8-Dimethanonaphthalene, 1,2,3,4,5,8-hexahydro-, (1«alpha»,4«alpha»,5«alpha»,8«alpha»)-

InChI: InChI=1S/C12H14/c1-2-8-5-7(1)-1-9-3-4-10-6-9)11(8)11/h1-2,7-10H,3-6H2/t7-,8-,9+,10+
InChIKey: QUKNLCCMKRXCSW-AXTSPUMRSA-N
Formula: C12H14
SMILES: C1=CC2CC1C1=C2C2CCC1C2
Mol. weight [g/mol]: 158.24
CAS: 73365-00-1

Physical Properties

Property code	Value	Unit	Source
gf	333.82	kJ/mol	Joback Method
hf	92.81	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
ie	7.87	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-3.17		Crippen Method
logp	2.919		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	509.20	K	Joback Method
tc	732.44	K	Joback Method
tf	323.32	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.56	J/mol×K	509.20	Joback Method
cpg	340.11	J/mol×K	546.41	Joback Method
cpg	357.14	J/mol×K	583.61	Joback Method
cpg	372.78	J/mol×K	620.82	Joback Method
cpg	387.20	J/mol×K	658.02	Joback Method
cpg	400.55	J/mol×K	695.23	Joback Method
cpg	412.97	J/mol×K	732.44	Joback Method

dvisc	0.0011801	Pa×s	323.32	Joback Method
dvisc	0.0015122	Pa×s	354.30	Joback Method
dvisc	0.0018621	Pa×s	385.28	Joback Method
dvisc	0.0022230	Pa×s	416.26	Joback Method
dvisc	0.0025895	Pa×s	447.24	Joback Method
dvisc	0.0029573	Pa×s	478.22	Joback Method
dvisc	0.0033233	Pa×s	509.20	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	https://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73365001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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