

1,4:5,8-Dimethanonaphthalene, 1,2,3,4,5,8-hexahydro-

InChI: InChI=1S/C12H14/c1-2-8-5-7(11)-9-3-6-10(-9)12(8)11/h1-2,7-10H,3-6H2/t7-,8-,9+,10+
(1«alpha»,4«alpha»,5«beta»,8«beta»)-
InChIKey: QUKNLCCMKRXCSW-IMSYWVGJSA-N

Formula: C12H14
SMILES: C1=CC2CC1C1=C2C2CCC1C2
Mol. weight [g/mol]: 158.24
CAS: 102340-97-6

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	7.40	eV	NIST Webbook
ie	7.80	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/molxK	509.20	Joback Method
cpg	400.55	J/molxK	695.23	Joback Method
cpg	387.20	J/molxK	658.02	Joback Method
cpg	372.78	J/molxK	620.82	Joback Method
cpg	357.14	J/molxK	583.61	Joback Method
cpg	340.11	J/molxK	546.41	Joback Method
cpg	412.97	J/molxK	732.44	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102340976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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