

1,4:5,8-Dimethanonaphthalene,1,4,4a,5,8,8a-hexal

Inchi:	InChI=1S/C12H14/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h1-4,7-12H,5-6H2/t7-,8+,9+,10-
InchiKey:	ZSJSPFJUHHVKQB-WAODVVSYSYSA-N
Formula:	C12H14
SMILES:	C1=CC2CC1C1C3C=CC(C3)C21
Mol. weight [g/mol]:	158.24
CAS:	1076-13-7

Physical Properties

Property code	Value	Unit	Source
gf	337.66	kJ/mol	Joback Method
hf	75.07	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
ie	8.08 ± 0.03	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.631		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	489.90	K	Joback Method
tc	710.29	K	Joback Method
tf	289.80	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.54	J/molxK	489.90	Joback Method
cpg	341.07	J/molxK	526.63	Joback Method
cpg	359.95	J/molxK	563.36	Joback Method
cpg	377.31	J/molxK	600.10	Joback Method
cpg	393.29	J/molxK	636.83	Joback Method
cpg	408.06	J/molxK	673.56	Joback Method
cpg	421.73	J/molxK	710.29	Joback Method
dvisc	0.0005230	Paxs	289.80	Joback Method

dvisc	0.0008339	Paxs	323.15	Joback Method
dvisc	0.0012184	Paxs	356.50	Joback Method
dvisc	0.0016684	Paxs	389.85	Joback Method
dvisc	0.0021742	Paxs	423.20	Joback Method
dvisc	0.0027258	Paxs	456.55	Joback Method
dvisc	0.0033138	Paxs	489.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1076137&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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