

1,4:5,8-Dimethanonaphthalene, decahydro-, (1 «alpha»,4 «alpha»,4a «alpha»,5 «alpha»,8 «alpha»

Inchi:	InChI=1S/C12H18/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h7-12H,1-6H2/t7-,8+,9+,10-,11+
InchiKey:	VSHDEZHNJCSDFY-WAODVVSYSYSA-N
Formula:	C12H18
SMILES:	C1CC2CC1C1C3CCC(C3)C21
Mol. weight [g/mol]:	162.27
CAS:	53862-33-2

Physical Properties

Property code	Value	Unit	Source
gf	277.74	kJ/mol	Joback Method
hf	-40.49	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	41.34	kJ/mol	Joback Method
ie	9.50 ± 0.03	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	3.079		Crippen Method
mcvol	136.500	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	491.58	K	Joback Method
tc	707.52	K	Joback Method
tf	288.28	K	Joback Method
vc	0.533	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.87	J/mol×K	491.58	Joback Method
cpg	376.79	J/mol×K	527.57	Joback Method
cpg	398.02	J/mol×K	563.56	Joback Method
cpg	417.69	J/mol×K	599.55	Joback Method
cpg	435.94	J/mol×K	635.54	Joback Method
cpg	452.90	J/mol×K	671.53	Joback Method
cpg	468.70	J/mol×K	707.52	Joback Method
dvisc	0.0006932	Paxs	288.28	Joback Method

dvisc	0.0010425	Paxs	322.16	Joback Method
dvisc	0.0014506	Paxs	356.05	Joback Method
dvisc	0.0019058	Paxs	389.93	Joback Method
dvisc	0.0023970	Paxs	423.81	Joback Method
dvisc	0.0029141	Paxs	457.70	Joback Method
dvisc	0.0034486	Paxs	491.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53862332&Units=SI
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

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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