

1,4:5,8-Dimethanonaphthalene, 1,2,3,4,4a,5,8,8a-octahydro-,

InChI: InChI=1S/C12H16/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h1-2,7-12H,3,6H2/t7-8+9-,0+
(1«alpha»,4«alpha»,4a«alpha»,5«beta»,8«beta»,8a«beta»)
InchiKey: XBFJAVXCNXDDBH-CJXDBHJISA-N

Formula: C12H16
SMILES: C1=CC2CC1C1C3CCC(C3)C21
Mol. weight [g/mol]: 160.26
CAS: 36012-52-9

Physical Properties

Property code	Value	Unit	Source
gf	307.70	kJ/mol	Joback Method
hf	17.29	kJ/mol	Joback Method
hfus	22.74	kJ/mol	Joback Method
hvap	41.63	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.65 ± 0.03	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.855		Crippen Method
mcvol	132.200	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	490.74	K	Joback Method
tc	708.89	K	Joback Method
tf	289.04	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.17	J/molxK	490.74	Joback Method
cpg	358.91	J/molxK	527.10	Joback Method
cpg	378.97	J/molxK	563.46	Joback Method
cpg	397.50	J/molxK	599.81	Joback Method
cpg	414.64	J/molxK	636.17	Joback Method
cpg	430.51	J/molxK	672.53	Joback Method

cpg	445.26	J/mol×K	708.89	Joback Method
dvisc	0.0006017	Paxs	289.04	Joback Method
dvisc	0.0009320	Paxs	322.66	Joback Method
dvisc	0.0013293	Paxs	356.27	Joback Method
dvisc	0.0017834	Paxs	389.89	Joback Method
dvisc	0.0022834	Paxs	423.51	Joback Method
dvisc	0.0028194	Paxs	457.12	Joback Method
dvisc	0.0033819	Paxs	490.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36012529&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

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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