

1,4:5,8-Dimethanonaphthalene, 1,4,5,8-tetrahydro-,

InChI: InChI=1S/C12H12/c1-2-8-5-7(1)-11-9-3-4-10-6-9-11(8)-11/h1-4,7-10H,5-6H2/t7-,8-,9+,10+
(1«alpha»,4«alpha»,5«alpha»,8«alpha»)-
InChIKey: KWPLEXGYQPSPLP-BECANLQMSA-N

Formula: C12H12
SMILES: C1=CC2CC1C1=C2C2C=CC1C2
Mol. weight [g/mol]: 156.22
CAS: 97253-51-5

Physical Properties

Property code	Value	Unit	Source
gf	363.78	kJ/mol	Joback Method
hf	150.59	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	44.16	kJ/mol	Joback Method
ie	7.84	eV	NIST Webbook
ie	7.40	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	2.695		Crippen Method
mcvol	123.600	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	508.36	K	Joback Method
tc	733.89	K	Joback Method
tf	324.08	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.28	J/molxK	508.36	Joback Method
cpg	377.29	J/molxK	696.30	Joback Method
cpg	365.07	J/molxK	658.71	Joback Method
cpg	351.82	J/molxK	621.13	Joback Method
cpg	337.37	J/molxK	583.54	Joback Method
cpg	321.58	J/molxK	545.95	Joback Method
cpg	388.64	J/molxK	733.89	Joback Method

dvisc	0.0032831	Paxs	508.36	Joback Method
dvisc	0.0028883	Paxs	477.65	Joback Method
dvisc	0.0024967	Paxs	446.93	Joback Method
dvisc	0.0021122	Paxs	416.22	Joback Method
dvisc	0.0017400	Paxs	385.51	Joback Method
dvisc	0.0013860	Paxs	354.79	Joback Method
dvisc	0.0010575	Paxs	324.08	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=C97253515&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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