

1,4,5,8-Tetrahydro-1,6-methanonaphthalene

Inchi:	InChI=1S/C11H14/c1-2-6-11-8-4-3-7-10(11,5-1)9-11/h1-4H,5-9H2
InchiKey:	WMBWQQJRLXTDPJ-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	C1=CCC23CC=CCC2(C1)C3
Mol. weight [g/mol]:	146.23
CAS:	27714-83-6

Physical Properties

Property code	Value	Unit	Source
chl	-6384.40 ± 5.40	kJ/mol	NIST Webbook
gf	256.44	kJ/mol	Joback Method
hf	102.09	kJ/mol	Joback Method
hfus	3.23	kJ/mol	Joback Method
hvap	38.75	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.063		Crippen Method
mcvol	124.670	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	483.31	K	Joback Method
tc	728.22	K	Joback Method
tf	314.07	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.95	J/mol×K	483.31	Joback Method
cpg	307.57	J/mol×K	524.13	Joback Method
cpg	324.92	J/mol×K	564.95	Joback Method
cpg	340.41	J/mol×K	605.76	Joback Method
cpg	354.45	J/mol×K	646.58	Joback Method
cpg	367.43	J/mol×K	687.40	Joback Method
cpg	379.75	J/mol×K	728.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27714836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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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