

1,2,3,10a-Tetrahydrophenanthrene

Inchi:	InChI=1S/C14H14/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1,3,5,7-10,12H,2,4,6H2
InchiKey:	HJBQLPMMTTXLSH-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	C1=CC2CCCC=C2c2ccccc21
Mol. weight [g/mol]:	182.26

Physical Properties

Property code	Value	Unit	Source
gf	325.08	kJ/mol	Joback Method
hf	150.48	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.897		Crippen Method
mcvol	154.040	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	316.17		NIST Webbook
rinpol	316.17		NIST Webbook
tb	581.37	K	Joback Method
tc	829.10	K	Joback Method
tf	333.60	K	Joback Method
vc	0.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.73	J/mol×K	581.37	Joback Method
cpg	395.20	J/mol×K	622.66	Joback Method
cpg	412.17	J/mol×K	663.95	Joback Method
cpg	427.77	J/mol×K	705.23	Joback Method
cpg	442.13	J/mol×K	746.52	Joback Method
cpg	455.37	J/mol×K	787.81	Joback Method
cpg	467.64	J/mol×K	829.10	Joback Method
dvisc	0.0018594	Paxs	333.60	Joback Method

dvisc	0.0013317	Paxs	374.90	Joback Method
dvisc	0.0010191	Paxs	416.19	Joback Method
dvisc	0.0008185	Paxs	457.49	Joback Method
dvisc	0.0006817	Paxs	498.78	Joback Method
dvisc	0.0005838	Paxs	540.08	Joback Method
dvisc	0.0005111	Paxs	581.37	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=R214354&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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