

1-Methyl-1,2,3,4-tetrahydrophenanthrene

Inchi:	InChI=1S/C15H16/c1-11-5-4-8-15-13(11)10-9-12-6-2-3-7-14(12)15/h2-3,6-7,9-11H,4-5,8H
InchiKey:	HEUMEXLOFIYOAS-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	CC1CCCc2c1ccc1ccccc21
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	323.87	kJ/mol	Joback Method
hf	118.37	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.280		Crippen Method
mcvol	168.130	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	1810.00		NIST Webbook
tb	609.23	K	Joback Method
tc	852.63	K	Joback Method
tf	357.39	K	Joback Method
vc	0.638	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.15	J/molxK	609.23	Joback Method
cpg	506.30	J/molxK	812.06	Joback Method
cpg	492.61	J/molxK	771.49	Joback Method
cpg	477.87	J/molxK	730.93	Joback Method
cpg	461.96	J/molxK	690.36	Joback Method
cpg	444.76	J/molxK	649.80	Joback Method
cpg	519.04	J/molxK	852.63	Joback Method
dvisc	0.0004911	Paxs	609.23	Joback Method
dvisc	0.0005582	Paxs	567.26	Joback Method

dvisc	0.0006475	Paxs	525.28	Joback Method
dvisc	0.0007707	Paxs	483.31	Joback Method
dvisc	0.0009483	Paxs	441.34	Joback Method
dvisc	0.0012188	Paxs	399.36	Joback Method
dvisc	0.0016615	Paxs	357.39	Joback Method

Sources

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=R578168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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