

9,10-Ethanoanthracene, 9,10-dihydro-

Other names:	Dibenzobicyclo[2.2.2]octadiene 1,4-endo-o-Phenylenenaphthalene, 1,2,3,4-tetrahydro- 9,10-Dihydro-9,10-ethanoanthracene
Inchi:	InChI=1S/C16H14/c1-2-6-12-11(5-1)15-9-10-16(12)14-8-4-3-7-13(14)15/h1-8,15-16H,9-10
InchiKey:	VPPCQVCZKDIGGG-UHFFFAOYSA-N
Formula:	C16H14
SMILES:	<chem>c1ccc2c(c1)C1CCC2c2ccccc21</chem>
Mol. weight [g/mol]:	206.28
CAS:	5675-64-9

Physical Properties

Property code	Value	Unit	Source
gf	435.10	kJ/mol	Joback Method
hf	234.47	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-4.58		Crippen Method
logp	4.058		Crippen Method
mcvol	167.060	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	633.74	K	Joback Method
tc	883.39	K	Joback Method
tf	390.88	K	Joback Method
vc	0.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.91	J/mol×K	633.74	Joback Method
cpg	513.61	J/mol×K	841.79	Joback Method
cpg	500.81	J/mol×K	800.18	Joback Method
cpg	487.13	J/mol×K	758.57	Joback Method

cpg	472.38	J/molxK	716.96	Joback Method
cpg	456.37	J/molxK	675.35	Joback Method
cpg	525.72	J/molxK	883.39	Joback Method
dvisc	0.0016202	Paxs	633.74	Joback Method
dvisc	0.0016775	Paxs	593.26	Joback Method
dvisc	0.0017457	Paxs	552.79	Joback Method
dvisc	0.0018282	Paxs	512.31	Joback Method
dvisc	0.0019297	Paxs	471.83	Joback Method
dvisc	0.0020577	Paxs	431.36	Joback Method
dvisc	0.0022236	Paxs	390.88	Joback Method

Sources

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=C5675649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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