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,9-1
InchiKey: VPPCQVCZKDIGGG-UHFFFAOYSA-N
Formula: C16H14
SMILES: c1ccc2c(c1)C1CCC2c2ccccc21
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	8.30	eV	NIST Webbook
ie	8.10	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.91	J/mol×K	633.74	Joback Method
cpg	456.37	J/mol×K	675.35	Joback Method
cpg	472.38	J/mol×K	716.96	Joback Method
cpg	487.13	J/mol×K	758.57	Joback Method

cpg	500.81	J/mol×K	800.18	Joback Method
cpg	513.61	J/mol×K	841.79	Joback Method
cpg	525.72	J/mol×K	883.39	Joback Method
dvisc	0.0022236	Pa×s	390.88	Joback Method
dvisc	0.0020577	Pa×s	431.36	Joback Method
dvisc	0.0019297	Pa×s	471.83	Joback Method
dvisc	0.0018282	Pa×s	512.31	Joback Method
dvisc	0.0017457	Pa×s	552.79	Joback Method
dvisc	0.0016775	Pa×s	593.26	Joback Method
dvisc	0.0016202	Pa×s	633.74	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5675649&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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