1,4-Methanoanthracene,1,4-dihydro-9,10-dimetho

Other names: Antrhracene, 1,4-dihydro-1,4-methano-9,10-dimethoxy-
Inchi: InChI=1S/C17H16O2/c1-18-16-12-5-3-4-6-13(12)17(19-2)15-11-8-7-10(9-11)14(15)16/h3
InchiKey: MVNKVWQSNVLBIV-UHFFFAOYSA-N
Formula: C17H16O2
SMILES: COc1c2c(c(OC)c3ccccc13)C1C=CC2C1
Mol. weight [g/mol]: 252.31
CAS: 52457-25-7

Physical Properties

Property code	Value	Unit	Source
gf	226.36	kJ/mol	Joback Method
hf	-67.39	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
ie	7.55	eV	NIST Webbook
log10ws	-5.11		Crippen Method
logp	3.998		Crippen Method
mcvol	192.890	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
tb	707.15	K	Joback Method
tc	938.29	K	Joback Method
tf	475.17	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.07	J/mol×K	707.15	Joback Method
cpg	554.72	J/mol×K	745.67	Joback Method
cpg	569.38	J/mol×K	784.20	Joback Method
cpg	583.15	J/mol×K	822.72	Joback Method
cpg	596.16	J/mol×K	861.25	Joback Method
cpg	608.50	J/mol×K	899.77	Joback Method
cpg	620.29	J/mol×K	938.29	Joback Method

dvisc	0.0020487	Pa×s	475.17	Joback Method
dvisc	0.0019397	Pa×s	513.83	Joback Method
dvisc	0.0018506	Pa×s	552.50	Joback Method
dvisc	0.0017764	Pa×s	591.16	Joback Method
dvisc	0.0017139	Pa×s	629.82	Joback Method
dvisc	0.0016604	Pa×s	668.49	Joback Method
dvisc	0.0016141	Pa×s	707.15	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=C52457257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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