trans-Phenanthrene, 9,10-dihydro-9,10-diol

Other names: 9,10-Phenanthrenediol, 9,10-dihydro- (E)-
Inchi: InChI=1S/C14H12O2/c15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16/h1-8,13-16H
InchiKey: MFXNBQWUTDDOKE-UHFFFAOYSA-N
Formula: C14H12O2
SMILES: OC1c2ccccc2-c2ccccc2C1O
Mol. weight [g/mol]: 212.24
CAS: 572-41-8

Physical Properties

Property code	Value	Unit	Source
gf	64.06	kJ/mol	Joback Method
hf	-128.01	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
ie	8.13	eV	NIST Webbook
log10ws	-4.18		Crippen Method
logp	2.434		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	2020.00		NIST Webbook
tb	765.20	K	Joback Method
tc	978.77	K	Joback Method
tf	464.28	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.64	J/mol×K	765.20	Joback Method
cpg	471.31	J/mol×K	800.79	Joback Method
cpg	481.29	J/mol×K	836.39	Joback Method
cpg	490.66	J/mol×K	871.98	Joback Method
cpg	499.49	J/mol×K	907.58	Joback Method
cpg	507.85	J/mol×K	943.17	Joback Method

cpg	515.83	J/mol×K	978.77	Joback Method
dvisc	0.0012437	Pa×s	464.28	Joback Method
dvisc	0.0005307	Pa×s	514.43	Joback Method
dvisc	0.0002635	Pa×s	564.59	Joback Method
dvisc	0.0001466	Pa×s	614.74	Joback Method
dvisc	0.0000892	Pa×s	664.89	Joback Method
dvisc	0.0000581	Pa×s	715.05	Joback Method
dvisc	0.0000401	Pa×s	765.20	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=C572418&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume