cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol

Inchi: InChI=1S/C15H14O2/c1-15(17)13-9-5-4-7-11(13)10-6-2-3-8-12(10)14(15)16/h2-9,14,16-

InchiKey: ADDCOOKVSJVBSM-LSDHHAIUSA-N

Formula: C15H14O2

SMILES: CC1(O)c2ccccc2-c2ccccc2C1O

Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	66.99	kJ/mol	Joback Method
hf	-133.41	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	86.50	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.608		Crippen Method
mcvol	175.570	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	788.32	K	Joback Method
tc	1005.45	K	Joback Method
tf	499.45	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.80	J/mol×K	788.32	Joback Method
cpg	520.80	J/mol×K	824.51	Joback Method
cpg	532.62	J/mol×K	860.70	Joback Method
cpg	544.41	J/mol×K	896.89	Joback Method
cpg	556.34	J/mol×K	933.07	Joback Method
cpg	568.58	J/mol×K	969.26	Joback Method
cpg	581.30	J/mol×K	1005.45	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=R109450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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