cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3,4-dimethoxy

Inchi: InChI=1S/C17H18O4/c1-17(19)12-7-5-4-6-10(12)14-11(16(17)18)8-9-13(20-2)15(14)21-3

InchiKey: SEDCUXLTUOHWJO-SJORKVTESA-N

Formula: C17H18O4

SMILES: COc1ccc2c(c1OC)-c1ccccc1C(C)(O)C2O

Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-145.43	kJ/mol	Joback Method
hf	-462.07	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	97.09	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	2.625		Crippen Method
mcvol	215.490	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	2460.00		NIST Webbook
tb	888.88	K	Joback Method
tc	1103.71	K	Joback Method
tf	591.49	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.51	J/mol×K	888.88	Joback Method
cpg	684.37	J/mol×K	924.68	Joback Method
cpg	698.16	J/mol×K	960.49	Joback Method
cpg	712.01	J/mol×K	996.29	Joback Method
cpg	726.04	J/mol×K	1032.10	Joback Method
cpg	740.39	J/mol×K	1067.90	Joback Method
cpg	755.16	J/mol×K	1103.71	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=R109465&Units=SI

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

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