5-(4-Methoxyphenyl)-10,11-dihydro-5H-dibenzo[a,

Inchi: InChI=1S/C22H20O2/c1-24-19-14-12-18(13-15-19)22(23)20-8-4-2-6-16(20)10-11-17-7-3
InchiKey: HQSHHWRBALRELU-UHFFFAOYSA-N
Formula: C22H20O2
SMILES: COc1ccc(C2(O)c3ccccc3CCc3ccccc32)cc1
Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	256.14	kJ/mol	Joback Method
hf	-18.64	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	91.23	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.078		Crippen Method
mcvol	250.440	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2661.00		NIST Webbook
ripol	3906.00		NIST Webbook
tb	919.32	K	Joback Method
tc	1166.34	K	Joback Method
tf	579.41	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.28	J/mol×K	919.32	Joback Method
cpg	796.92	J/mol×K	960.49	Joback Method
cpg	814.59	J/mol×K	1001.66	Joback Method
cpg	832.52	J/mol×K	1042.83	Joback Method
cpg	850.97	J/mol×K	1084.00	Joback Method
cpg	870.20	J/mol×K	1125.17	Joback Method
cpg	890.45	J/mol×K	1166.34	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=R537701&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume