5-(4-Chlorophenyl)-10,11-dihydro-5H-dibenzo[a,d]

Inchi: InChI=1S/C21H17ClO/c22-18-13-11-17(12-14-18)21(23)19-7-3-1-5-15(19)9-10-16-6-2-4-
InchiKey: OFXNZLUQVYCHQK-UHFFFAOYSA-N
Formula: C21H17ClO
SMILES: OC1(c2ccc(Cl)cc2)c2ccccc2CCc2ccccc21
Mol. weight [g/mol]: 320.81

Physical Properties

Property code	Value	Unit	Source
gf	340.79	kJ/mol	Joback Method
hf	118.48	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.723		Crippen Method
mcvol	242.720	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
ripol	3822.00		NIST Webbook
tb	911.45	K	Joback Method
tc	1167.18	K	Joback Method
tf	575.83	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.71	J/mol×K	911.45	Joback Method
cpg	733.59	J/mol×K	954.07	Joback Method
cpg	750.70	J/mol×K	996.69	Joback Method
cpg	768.36	J/mol×K	1039.32	Joback Method
cpg	786.85	J/mol×K	1081.94	Joback Method
cpg	806.50	J/mol×K	1124.56	Joback Method
cpg	827.61	J/mol×K	1167.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537692&Units=SI
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

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