11-(4-Chlorophenyl)-6,11-dihydrodibenzo[b,e]oxe

Inchi: InChI=1S/C20H15ClO2/c21-16-11-9-15(10-12-16)20(22)17-6-2-1-5-14(17)13-23-19-8-4-3

InchiKey: JPJOKKPGJCCQQO-UHFFFAOYSA-N

Formula: C20H15ClO2

SMILES: OC1(c2ccc(Cl)cc2)c2ccccc2COc2ccccc21

Mol. weight [g/mol]: 322.79

Physical Properties

Property code	Value	Unit	Source
gf	246.25	kJ/mol	Joback Method
hf	7.12	kJ/mol	Joback Method
hfus	36.61	kJ/mol	Joback Method
hvap	93.26	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.517		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	2598.00		NIST Webbook
ripol	3923.00		NIST Webbook
tb	915.52	K	Joback Method
tc	1172.51	K	Joback Method
tf	591.13	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.27	J/mol×K	915.52	Joback Method
cpg	704.20	J/mol×K	958.35	Joback Method
cpg	720.44	J/mol×K	1001.18	Joback Method
cpg	737.27	J/mol×K	1044.02	Joback Method
cpg	755.00	J/mol×K	1086.85	Joback Method
cpg	773.94	J/mol×K	1129.68	Joback Method
cpg	794.37	J/mol×K	1172.51	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=R537667&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume