Benzo[b]benzo[3,4]cyclobuta[1,2-e][1,4]dioxin, 4b,10a-dihydro-4b-phenyl-

Inchi: InChI=1S/C20H14O2/c1-2-8-14(9-3-1)20-16-11-5-4-10-15(16)19(20)21-17-12-6-7-13-18(
Inchikey: PSQTZUPHZFJNTH-UHFFFAOYSA-N
Formula: C20H14O2
SMILES: c1ccc(C23Oc4ccccc4OC2c2ccccc23)cc1
Mol. weight [g/mol]: 286.32
CAS: 53486-88-7

Physical Properties

Property code	Value	Unit	Source
gf	403.46	kJ/mol	Joback Method
hf	139.68	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	75.62	kJ/mol	Joback Method
ie	7.58 ± 0.02	eV	NIST Webbook
log10ws	-5.42		Crippen Method
logp	4.456		Crippen Method
mcvol	211.400	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	806.08	K	Joback Method
tc	1082.32	K	Joback Method
tf	539.42	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.55	J/mol×K	806.08	Joback Method
cpg	635.63	J/mol×K	852.12	Joback Method
cpg	652.56	J/mol×K	898.16	Joback Method
cpg	669.80	J/mol×K	944.20	Joback Method
cpg	687.82	J/mol×K	990.24	Joback Method
cpg	707.08	J/mol×K	1036.28	Joback Method
cpg	728.04	J/mol×K	1082.32	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=C53486887&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume