2,3-Diphenylbenzo-1,4-dioxin

Other names: 1,4-Benzodioxin,2,3-diphenyl-
Inchi: InChI=1S/C20H14O2/c1-3-9-15(10-4-1)19-20(16-11-5-2-6-12-16)22-18-14-8-7-13-17(18)21-19
InchiKey: SORQOTLULXSBOM-UHFFFAOYSA-N
Formula: C20H14O2
SMILES: c1ccc(C2=C(c3ccccc3)Oc3ccccc3O2)cc1
Mol. weight [g/mol]: 286.32
CAS: 75694-46-1

Physical Properties

Property code	Value	Unit	Source
gf	339.94	kJ/mol	Joback Method
hf	99.81	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
ie	7.08 ± 0.02	eV	NIST Webbook
log10ws	-6.01		Crippen Method
logp	4.984		Crippen Method
mcvol	217.960	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	820.72	K	Joback Method
tc	1097.21	K	Joback Method
tf	504.54	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.11	J/mol×K	820.72	Joback Method
cpg	632.32	J/mol×K	866.80	Joback Method
cpg	646.14	J/mol×K	912.88	Joback Method
cpg	658.72	J/mol×K	958.97	Joback Method
cpg	670.27	J/mol×K	1005.05	Joback Method
cpg	680.96	J/mol×K	1051.13	Joback Method
cpg	690.98	J/mol×K	1097.21	Joback Method

dvisc	0.0009451	Pa×s	504.54	Joback Method
dvisc	0.0005979	Pa×s	557.24	Joback Method
dvisc	0.0004093	Pa×s	609.93	Joback Method
dvisc	0.0002977	Pa×s	662.63	Joback Method
dvisc	0.0002269	Pa×s	715.33	Joback Method
dvisc	0.0001795	Pa×s	768.02	Joback Method
dvisc	0.0001463	Pa×s	820.72	Joback Method

Sources

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=C75694461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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