2,6-Methano-1,4-benzodioxocin-5(6h)-one, 2,3-dihydro-6-phenyl-

Inchi: InChI=1S/C17H14O3/c18-16-17(12-6-2-1-3-7-12)10-13(11-19-16)20-15-9-5-4-8-14(15)17

InchiKey: NLBWDTCEJFEMED-UHFFFAOYSA-N

Formula: C17H14O3

SMILES: O=C1OCC2CC1(c1ccccc1)c1ccccc1O2

Mol. weight [g/mol]: 266.29

CAS: 93321-57-4

Physical Properties

Property code	Value	Unit	Source
gf	116.53	kJ/mol	Joback Method
hf	-179.64	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.681		Crippen Method
mcvol	194.460	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	786.41	K	Joback Method
tc	1066.14	K	Joback Method
tf	524.33	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.72	J/mol×K	786.41	Joback Method
cpg	601.82	J/mol×K	833.03	Joback Method
cpg	619.19	J/mol×K	879.65	Joback Method
cpg	636.17	J/mol×K	926.28	Joback Method
cpg	653.10	J/mol×K	972.90	Joback Method
cpg	670.30	J/mol×K	1019.52	Joback Method
cpg	688.12	J/mol×K	1066.14	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=C93321574&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume