6-(Benzo[d][1,3]dioxol-5-yl)hexa-3,5-dien-2-one

Inchi: InChI=1S/C13H12O3/c1-10(14)4-2-3-5-11-6-7-12-13(8-11)16-9-15-12/h2-8H,9H2,1H3/b4
InchiKey: IDYPDRFMVHXYEC-ZUVMSYQZSA-N
Formula: C13H12O3
SMILES: CC(=O)C=CC=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 216.23
CAS: 17172-93-9

Physical Properties

Property code	Value	Unit	Source
gf	79.47	kJ/mol	Joback Method
hf	-147.06	kJ/mol	Joback Method
hfus	37.71	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.574		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	2055.20		NIST Webbook
rinpol	2055.20		NIST Webbook
tb	660.98	K	Joback Method
tc	896.30	K	Joback Method
tf	402.82	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.51	J/mol×K	660.98	Joback Method
cpg	473.07	J/mol×K	857.08	Joback Method
cpg	463.24	J/mol×K	817.86	Joback Method
cpg	452.79	J/mol×K	778.64	Joback Method
cpg	441.59	J/mol×K	739.42	Joback Method
cpg	429.54	J/mol×K	700.20	Joback Method
cpg	482.38	J/mol×K	896.30	Joback Method

dvisc	0.0002922	Pa×s	660.98	Joback Method
dvisc	0.0003550	Pa×s	617.95	Joback Method
dvisc	0.0004441	Pa×s	574.93	Joback Method
dvisc	0.0005762	Pa×s	531.90	Joback Method
dvisc	0.0007825	Pa×s	488.87	Joback Method
dvisc	0.0011273	Pa×s	445.85	Joback Method
dvisc	0.0017559	Pa×s	402.82	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=C17172939&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume