Syn-7,14-dihydro-1,6:8,13-bismethano[14]annuler

Inchi: InChI=1S/C16H12O2/c17-15-11-5-1-2-6-12(9-11)16(18)14-8-4-3-7-13(15)10-14/h1-8H,9-
InchiKey: KZGAVZQBBXMVGS-UHFFFAOYSA-N
Formula: C16H12O2
SMILES: O=C1C2=CC=CC=C(C2)C(=O)C2=CC=CC=C1C2
Mol. weight [g/mol]: 236.27
CAS: 104713-92-0

Physical Properties

Property code	Value	Unit	Source
gf	100.58	kJ/mol	Joback Method
hf	-111.87	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-3.89		Crippen Method
logp	2.764		Crippen Method
mcvol	181.060	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	780.12	K	Joback Method
tc	1058.83	K	Joback Method
tf	503.06	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.40	J/mol×K	780.12	Joback Method
cpg	528.64	J/mol×K	826.57	Joback Method
cpg	543.21	J/mol×K	873.02	Joback Method
cpg	556.15	J/mol×K	919.48	Joback Method
cpg	567.47	J/mol×K	965.93	Joback Method
cpg	577.22	J/mol×K	1012.38	Joback Method
cpg	585.42	J/mol×K	1058.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104713920&Units=SI
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

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