5,8-Dihydro-2-phenyl-5,8-ethano-1,4-naphthoquin

Inchi: InChI=1S/C18H14O2/c19-15-10-14(11-4-2-1-3-5-11)18(20)17-13-8-6-12(7-9-13)16(15)17
InchiKey: LHKZLRTYJXOLJF-UHFFFAOYSA-N
Formula: C18H14O2
SMILES: O=C1C=C(c2ccccc2)C(=O)C2=C1C1C=CC2CC1
Mol. weight [g/mol]: 262.30
CAS: 93655-07-3

Physical Properties

Property code	Value	Unit	Source
gf	182.56	kJ/mol	Joback Method
hf	-94.53	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.114		Crippen Method
mcvol	198.380	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	823.68	K	Joback Method
tc	1098.26	K	Joback Method
tf	542.82	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.19	J/mol×K	823.68	Joback Method
cpg	622.97	J/mol×K	869.44	Joback Method
cpg	638.19	J/mol×K	915.21	Joback Method
cpg	651.93	J/mol×K	960.97	Joback Method
cpg	664.31	J/mol×K	1006.74	Joback Method
cpg	675.42	J/mol×K	1052.50	Joback Method
cpg	685.37	J/mol×K	1098.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93655073&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

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