5,8-Dihydro-2-phenyl-5,8-methano-1,4-naphthoqu

Inchi: InChI=1S/C17H12O2/c18-14-9-13(10-4-2-1-3-5-10)17(19)16-12-7-6-11(8-12)15(14)16/h1
InchiKey: BKBUDOUPSBILIX-UHFFFAOYSA-N
Formula: C17H12O2
SMILES: O=C1C=C(c2ccccc2)C(=O)C2=C1C1C=CC2C1
Mol. weight [g/mol]: 248.28
CAS: 93327-67-4

Physical Properties

Property code	Value	Unit	Source
gf	186.24	kJ/mol	Joback Method
hf	-67.73	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	67.46	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.724		Crippen Method
mcvol	184.290	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	796.53	K	Joback Method
tc	1069.58	K	Joback Method
tf	535.07	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.63	J/mol×K	796.53	Joback Method
cpg	563.66	J/mol×K	842.04	Joback Method
cpg	578.29	J/mol×K	887.55	Joback Method
cpg	591.65	J/mol×K	933.05	Joback Method
cpg	603.83	J/mol×K	978.56	Joback Method
cpg	614.96	J/mol×K	1024.07	Joback Method
cpg	625.13	J/mol×K	1069.58	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=C93327674&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