1,4,4a,8a-Tetrahydro-1,4-methanonaphthalene-5,8

Other names: 1,4,4-«alpha»,8-«alpha»-Tetrahydro-endo-1,4-methanonaphthalene-5,8-dione
Cyclopentadienebenzoquinone
1,4-Methanonaphthalene-5,8-dione, 1,4,4a,8a-tetrahydro-
1,4,4-alpha,8-alpha-Tetrahydro-endo-1,4-methanonaphthalene-5,8-dione
Inchi: InChI=1S/C11H10O2/c12-8-3-4-9(13)11-7-2-1-6(5-7)10(8)11/h1-4,6-7,10-11H,5H2
InchiKey: FQLRTGXTYFCECH-UHFFFAOYSA-N
Formula: C11H10O2
SMILES: O=C1C=CC(=O)C2C3C=CC(C3)C12
Mol. weight [g/mol]: 174.20
CAS: 1200-89-1

Physical Properties

Property code	Value	Unit	Source
chs	-5593.60 ± 5.40	kJ/mol	NIST Webbook
chs	-5606.89	kJ/mol	NIST Webbook
gf	6.82	kJ/mol	Joback Method
hf	-244.47	kJ/mol	Joback Method
hfs	-150.90	kJ/mol	NIST Webbook
hfus	16.99	kJ/mol	Joback Method
hvap	48.93	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.133		Crippen Method
mcvol	127.810	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	609.13	K	Joback Method
tc	863.79	K	Joback Method
tf	394.23	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.30	J/mol×K	609.13	Joback Method
cpg	370.02	J/mol×K	651.57	Joback Method

cpg	386.47	J/mol×K	694.02	Joback Method
cpg	401.70	J/mol×K	736.46	Joback Method
cpg	415.74	J/mol×K	778.90	Joback Method
cpg	428.67	J/mol×K	821.35	Joback Method
cpg	440.52	J/mol×K	863.79	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1200891&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase 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