5,12-Dihydro-5,6,11,12-tetraphenyl-5,12-epidioxy naphthacene

Inchi: InChI=1S/C42H28O2/c1-5-17-29(18-6-1)37-33-25-13-14-26-34(33)38(30-19-7-2-8-20-30)42(44-43-37,31-21-9-3-10-22-31)32-23-11-4-12-24-32/h1-28H

InchiKey: AQMPDRUEYIQQCY-UHFFFAOYSA-N

Formula: C42H28O2

SMILES: c1ccc(-c2c3c(c(-c4ccccc4)c4ccccc24)C2(c4ccccc4)OOC3(c3ccccc3)c3ccccc32)cc1

Mol. weight [g/mol]: 564.67

CAS: 32287-37-9

Physical Properties

Property code	Value	Unit	Source
chs	-21046.00 ± 21.00	kJ/mol	NIST Webbook
gf	998.20	kJ/mol	Joback Method
hf	567.09	kJ/mol	Joback Method
hfs	517.00 ± 21.00	kJ/mol	NIST Webbook
hfus	67.69	kJ/mol	Joback Method
hvap	133.89	kJ/mol	Joback Method
log10ws	-13.76		Crippen Method
logp	10.033		Crippen Method
mcvol	430.640	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
tb	1423.64	K	Joback Method
tc	1749.02	K	Joback Method
tf	960.78	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1906.54	J/mol×K	1423.64	Joback Method
cpg	2020.22	J/mol×K	1477.87	Joback Method
cpg	2148.86	J/mol×K	1532.10	Joback Method
cpg	2293.82	J/mol×K	1586.33	Joback Method
cpg	2456.49	J/mol×K	1640.56	Joback Method
cpg	2638.24	J/mol×K	1694.79	Joback Method
cpg	2840.44	J/mol×K	1749.02	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=C32287379&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