Bisnaphtho[1',2':5,6]phenanthro[3,4-c:4',3'-g]phen

Inchi: InChI=1S/C54H30/c1-3-7-43-31(5-1)9-11-33-13-15-35-17-19-37-21-23-39-25-27-41-29-3
InchiKey: FDSRORWATQEJOV-UHFFFAOYSA-N
Formula: C54H30
SMILES: c1ccc2c(c1)ccc1ccc3ccc4ccc5ccc6ccc7ccc8ccc9ccc%10ccc%11ccc%12ccccc%12c%11
Mol. weight [g/mol]: 678.82
CAS: 24386-06-9

Physical Properties

Property code	Value	Unit	Source
gf	1690.08	kJ/mol	Joback Method
hf	1245.31	kJ/mol	Joback Method
hfus	89.61	kJ/mol	Joback Method
hvap	165.04	kJ/mol	Joback Method
ie	6.91	eV	NIST Webbook
log10ws	-23.13		Crippen Method
logp	15.525		Crippen Method
mcvol	514.440	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
tb	1744.14	K	Joback Method
tc	2165.50	K	Joback Method
tf	1254.88	K	Joback Method
vc	2.015	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2786.64	J/mol×K	1744.14	Joback Method
cpg	3035.52	J/mol×K	1814.37	Joback Method
cpg	3319.26	J/mol×K	1884.59	Joback Method
cpg	3640.67	J/mol×K	1954.82	Joback Method
cpg	4002.57	J/mol×K	2025.05	Joback Method
cpg	4407.78	J/mol×K	2095.27	Joback Method
cpg	4859.12	J/mol×K	2165.50	Joback Method
dvisc	0.0594564	Pa×s	1254.88	Joback Method

dvisc	0.0558309	Pa×s	1336.42	Joback Method
dvisc	0.0528073	Pa×s	1417.97	Joback Method
dvisc	0.0502508	Pa×s	1499.51	Joback Method
dvisc	0.0480635	Pa×s	1581.05	Joback Method
dvisc	0.0461725	Pa×s	1662.60	Joback Method
dvisc	0.0445227	Pa×s	1744.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24386069&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
dvisc:	Dynamic viscosity
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