Dinaphtho-[2,1,8-c,d,a:2',1',8'-nop]heptacene

Other names: Dinaphtho[2,1,8-c1d1a:2',1',8'-nop]heptacene
Inchi: InChI=1S/C42H22/c1-3-23-7-9-27-15-33-19-29-18-32-22-38-34(16-28-10-8-24-4-2-6-26-
InchiKey: IQAQPYAQWJUAGG-UHFFFAOYSA-N
Formula: C42H22
SMILES: c1cc2ccc3cc4cc5cc6cc7c(cc6cc5cc4c4ccc(c1)c2c34)cc1ccc2cccc3ccc7c1c23
Mol. weight [g/mol]: 526.62
CAS: 190-09-0

Physical Properties

Property code	Value	Unit	Source
gf	1383.48	kJ/mol	Joback Method
hf	1042.87	kJ/mol	Joback Method
hfus	71.22	kJ/mol	Joback Method
hvap	132.45	kJ/mol	Joback Method
ie	6.22	eV	NIST Webbook
log10ws	-18.35		Crippen Method
logp	12.094		Crippen Method
mcvol	392.880	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
tb	1406.26	K	Joback Method
tc	1722.20	K	Joback Method
tf	1041.76	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.00	J/mol×K	1406.26	Joback Method
cpg	2115.95	J/mol×K	1669.55	Joback Method
cpg	1980.30	J/mol×K	1616.89	Joback Method
cpg	1859.15	J/mol×K	1564.23	Joback Method
cpg	1751.42	J/mol×K	1511.57	Joback Method
cpg	1656.06	J/mol×K	1458.92	Joback Method
cpg	2267.15	J/mol×K	1722.20	Joback Method

dvisc	0.1356750	Pa×s	1406.26	Joback Method
dvisc	0.1365476	Pa×s	1345.51	Joback Method
dvisc	0.1375092	Pa×s	1284.76	Joback Method
dvisc	0.1385740	Pa×s	1224.01	Joback Method
dvisc	0.1397597	Pa×s	1163.26	Joback Method
dvisc	0.1410878	Pa×s	1102.51	Joback Method
dvisc	0.1425859	Pa×s	1041.76	Joback Method

Sources

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=C190090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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