Dinaphtho[8,1,2-abc!2',1',8'-efg]coronene

Other names: Dinaphtho[8,1,2-abc:2',1',8'-efg]coronene
Inchi: InChI=1S/C36H16/c1-3-17-9-13-25-26-14-10-18-4-2-6-22-24-16-12-20-8-7-19-11-15-23-
InchiKey: IALDVUQRLRCKEF-UHFFFAOYSA-N
Formula: C36H16
SMILES: c1cc2ccc3c4ccc5cccc6c7ccc8ccc9ccc%10c(c1)c2c3c1c%10c9c8c7c1c4c56
Mol. weight [g/mol]: 448.51
CAS: 122677-68-3

Physical Properties

Property code	Value	Unit	Source
gf	1315.68	kJ/mol	Joback Method
hf	1030.33	kJ/mol	Joback Method
hfus	64.62	kJ/mol	Joback Method
hvap	117.18	kJ/mol	Joback Method
log10ws	-16.59		Crippen Method
logp	10.408		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
tb	1245.88	K	Joback Method
tc	1533.31	K	Joback Method
tf	992.98	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.15	J/mol×K	1245.88	Joback Method
cpg	1215.75	J/mol×K	1293.79	Joback Method
cpg	1281.69	J/mol×K	1341.69	Joback Method
cpg	1356.83	J/mol×K	1389.60	Joback Method
cpg	1442.05	J/mol×K	1437.50	Joback Method
cpg	1538.20	J/mol×K	1485.41	Joback Method
cpg	1646.14	J/mol×K	1533.31	Joback Method
dvisc	1.7231260	Pa×s	992.98	Joback Method

dvisc	1.8218221	Pa×s	1035.13	Joback Method
dvisc	1.9177944	Pa×s	1077.28	Joback Method
dvisc	2.0110325	Pa×s	1119.43	Joback Method
dvisc	2.1015508	Pa×s	1161.58	Joback Method
dvisc	2.1893823	Pa×s	1203.73	Joback Method
dvisc	2.2745745	Pa×s	1245.88	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=C122677683&Units=SI

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
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