Dinaphtho[3,2,1-fg!3',2',1'-qr]pentacene

Other names: Dinaphtho[3,2,1-fg:3',2',1'-qr]pentacene
Inchi: InChI=1S/C36H20/c1-5-13-25-21(9-1)19-31-33-27-15-7-4-12-24(27)18-30-26-14-6-2-10-
InchiKey: WXRUBTMWQFFGIZ-UHFFFAOYSA-N
Formula: C36H20
SMILES: c1ccc2c(c1)cc1c3c4ccccc4cc4c5ccccc5cc(c5c6ccccc6cc2c15)c43
Mol. weight [g/mol]: 452.54
CAS: 128721-00-6

Physical Properties

Property code	Value	Unit	Source
gf	1144.68	kJ/mol	Joback Method
hf	852.97	kJ/mol	Joback Method
hfus	59.44	kJ/mol	Joback Method
hvap	115.12	kJ/mol	Joback Method
log10ws	-15.32		Crippen Method
logp	10.350		Crippen Method
mcvol	342.960	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	1228.76	K	Joback Method
tc	1519.31	K	Joback Method
tf	877.42	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.13	J/mol×K	1228.76	Joback Method
cpg	1214.90	J/mol×K	1277.19	Joback Method
cpg	1258.52	J/mol×K	1325.61	Joback Method
cpg	1307.64	J/mol×K	1374.04	Joback Method
cpg	1362.92	J/mol×K	1422.46	Joback Method
cpg	1425.02	J/mol×K	1470.89	Joback Method
cpg	1494.62	J/mol×K	1519.31	Joback Method
dvisc	0.0228438	Pa×s	877.42	Joback Method

dvisc	0.0217885	Pa×s	935.98	Joback Method
dvisc	0.0208980	Pa×s	994.53	Joback Method
dvisc	0.0201371	Pa×s	1053.09	Joback Method
dvisc	0.0194799	Pa×s	1111.65	Joback Method
dvisc	0.0189069	Pa×s	1170.20	Joback Method
dvisc	0.0184030	Pa×s	1228.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128721006&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

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