Bisbenzo[5,6]phenanthro[3,4-c:4',3'-g]phenanthre

Inchi: InChI=1S/C46H26/c1-3-7-37-27(5-1)9-11-29-13-15-31-17-19-33-21-23-35-25-26-36-24-2
InchiKey: BWVBAFLXLKBSEB-UHFFFAOYSA-N
Formula: C46H26
SMILES: c1ccc2c(c1)ccc1ccc3ccc4ccc5ccc6ccc7ccc8ccc9ccc%10ccccc%10c9c8c7c6c5c4c3c12
Mol. weight [g/mol]: 578.70
CAS: 57468-45-8

Physical Properties

Property code	Value	Unit	Source
gf	1428.68	kJ/mol	Joback Method
hf	1051.23	kJ/mol	Joback Method
hfus	75.63	kJ/mol	Joback Method
hvap	142.62	kJ/mol	Joback Method
ie	6.95	eV	NIST Webbook
log10ws	-19.52		Crippen Method
logp	13.219		Crippen Method
mcvol	440.640	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
tb	1513.18	K	Joback Method
tc	1853.19	K	Joback Method
tf	1074.28	K	Joback Method
vc	1.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1858.00	J/mol×K	1513.18	Joback Method
cpg	1961.07	J/mol×K	1569.85	Joback Method
cpg	2077.85	J/mol×K	1626.52	Joback Method
cpg	2209.60	J/mol×K	1683.18	Joback Method
cpg	2357.58	J/mol×K	1739.85	Joback Method
cpg	2523.04	J/mol×K	1796.52	Joback Method
cpg	2707.23	J/mol×K	1853.19	Joback Method
dvisc	0.0247104	Pa×s	1074.28	Joback Method

dvisc	0.0229597	Pa×s	1147.43	Joback Method
dvisc	0.0215218	Pa×s	1220.58	Joback Method
dvisc	0.0203220	Pa×s	1293.73	Joback Method
dvisc	0.0193073	Pa×s	1366.88	Joback Method
dvisc	0.0184389	Pa×s	1440.03	Joback Method
dvisc	0.0176881	Pa×s	1513.18	Joback Method

Sources

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=C57468458&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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