Dibenzo[a,jk]phenanthro[8,9,10,12-cdefgh]pyrantl

Inchi: InChI=1S/C44H20/c1-3-9-25-23(7-1)27-11-5-13-29-31-17-18-32-30-14-6-12-28-24-8-2-4-
InchiKey: ZZBAIFNSSHILSC-UHFFFAOYSA-N
Formula: C44H20
SMILES: c1ccc2c(c1)c1cccc3c4ccc5c6cccc7c8ccccc8c8cc9ccc%10cc2c(c13)c1c%10c9c(c8c76)c5
Mol. weight [g/mol]: 548.63
CAS: 70346-75-7

Physical Properties

Property code	Value	Unit	Source
gf	1577.08	kJ/mol	Joback Method
hf	1224.41	kJ/mol	Joback Method
hfus	78.60	kJ/mol	Joback Method
hvap	139.60	kJ/mol	Joback Method
ie	6.79 ± 0.02	eV	NIST Webbook
log10ws	-20.20		Crippen Method
logp	12.714		Crippen Method
mcvol	395.040	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
tb	1476.84	K	Joback Method
tc	1809.42	K	Joback Method
tf	1173.58	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1829.87	J/mol×K	1476.84	Joback Method
cpg	2742.59	J/mol×K	1753.99	Joback Method
cpg	2515.35	J/mol×K	1698.56	Joback Method
cpg	2312.00	J/mol×K	1643.13	Joback Method
cpg	2131.01	J/mol×K	1587.70	Joback Method
cpg	1970.81	J/mol×K	1532.27	Joback Method
cpg	2995.28	J/mol×K	1809.42	Joback Method
dvisc	7.9362824	Pa×s	1476.84	Joback Method

dvisc	7.6920672	Pa×s	1426.30	Joback Method
dvisc	7.4382649	Pa×s	1375.75	Joback Method
dvisc	7.1744515	Pa×s	1325.21	Joback Method
dvisc	6.9002058	Pa×s	1274.67	Joback Method
dvisc	6.6151181	Pa×s	1224.12	Joback Method
dvisc	6.3188025	Pa×s	1173.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70346757&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