

Benzo[g]phenanthro[3,4-c:6,5-c']diphenanthrene

Other names:	Benzo[g]phenanthro[3,4-c:6,5-c']diphenanthrene
Inchi:	InChI=1S/C42H24/c1-3-7-34-25(5-1)9-11-27-13-15-29-17-19-31-21-23-33-24-22-32-20-1
InchiKey:	DZNSHUKRWMZMLS-UHFFFAOYSA-N
Formula:	C42H24
SMILES:	c1ccc2c(c1)ccc1ccc3ccc4ccc5ccc6ccc7ccc8ccc9ccccc9c8c7c6c5c4c3c12
Mol. weight [g/mol]:	528.64
CAS:	57520-29-3

Physical Properties

Property code	Value	Unit	Source
gf	1297.98	kJ/mol	Joback Method
hf	954.19	kJ/mol	Joback Method
hfus	68.64	kJ/mol	Joback Method
hvap	131.42	kJ/mol	Joback Method
ie	6.99	eV	NIST Webbook
log10ws	-17.71		Crippen Method
logp	12.065		Crippen Method
mcvol	403.740	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
tb	1397.70	K	Joback Method
tc	1712.86	K	Joback Method
tf	983.98	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.99	J/molxK	1397.70	Joback Method
cpg	1607.01	J/molxK	1450.23	Joback Method
cpg	1681.64	J/molxK	1502.75	Joback Method
cpg	1765.78	J/molxK	1555.28	Joback Method
cpg	1860.33	J/molxK	1607.80	Joback Method
cpg	1966.22	J/molxK	1660.33	Joback Method
cpg	2084.34	J/molxK	1712.86	Joback Method

dvisc	0.0160267	Paxs	983.98	Joback Method
dvisc	0.0147862	Paxs	1052.93	Joback Method
dvisc	0.0137775	Paxs	1121.89	Joback Method
dvisc	0.0129431	Paxs	1190.84	Joback Method
dvisc	0.0122427	Paxs	1259.79	Joback Method
dvisc	0.0116472	Paxs	1328.75	Joback Method
dvisc	0.0111354	Paxs	1397.70	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=C57520293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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