

Benzo[*rst*]pyreno[1,10,9-*cde*]pentaphene

Inchi:	InChI=1S/C36H18/c1-2-6-24-22(4-1)18-23-13-15-29-34-26(17-16-25(24)31(23)34)27-14-
InchiKey:	PAOYPZXOQIZBHE-UHFFFAOYSA-N
Formula:	C36H18
SMILES:	<chem>c1ccc2c(c1)cc1ccc3c4c(ccc2c14)c1ccc2ccc4ccc5cccc6c5c4c2c1c63</chem>
Mol. weight [g/mol]:	450.53
CAS:	117740-28-0

Physical Properties

Property code	Value	Unit	Source
gf	1230.18	kJ/mol	Joback Method
hf	941.65	kJ/mol	Joback Method
hfus	62.03	kJ/mol	Joback Method
hvap	116.15	kJ/mol	Joback Method
log10ws	-15.96		Crippen Method
logp	10.379		Crippen Method
mcvol	332.100	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	1237.32	K	Joback Method
tc	1526.05	K	Joback Method
tf	935.20	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.67	J/mol×K	1237.32	Joback Method
cpg	1478.54	J/mol×K	1477.93	Joback Method
cpg	1399.76	J/mol×K	1429.81	Joback Method
cpg	1329.84	J/mol×K	1381.68	Joback Method
cpg	1268.03	J/mol×K	1333.56	Joback Method
cpg	1213.56	J/mol×K	1285.44	Joback Method
cpg	1566.95	J/mol×K	1526.05	Joback Method
dvisc	0.2034462	Paxs	1237.32	Joback Method
dvisc	0.2010371	Paxs	1186.97	Joback Method

dvisc	0.1984470	Paxs	1136.61	Joback Method
dvisc	0.1956549	Paxs	1086.26	Joback Method
dvisc	0.1926365	Paxs	1035.91	Joback Method
dvisc	0.1893636	Paxs	985.55	Joback Method
dvisc	0.1858032	Paxs	935.20	Joback Method

Sources

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=C117740280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
mccvol:	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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