

Benzo[a]perylene

Inchi:	InChI=1S/C24H14/c1-2-10-18-16(6-1)14-17-9-5-12-20-19-11-3-7-15-8-4-13-21(22(15)19)
InchiKey:	JDPBLCQVGZLACA-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	<chem>c1ccc2c(c1)cc1cccc3c4cccc5cccc(c54)c2c13</chem>
Mol. weight [g/mol]:	302.37
CAS:	191-85-5

Physical Properties

Property code	Value	Unit	Source
gf	752.58	kJ/mol	Joback Method
hf	561.85	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
ie	6.71	eV	NIST Webbook
ie	6.71	eV	NIST Webbook
log10ws	-9.91		Crippen Method
logp	6.890		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	537.04		NIST Webbook
rinpol	542.80		NIST Webbook
rinpol	537.04		NIST Webbook
rinpol	542.80		NIST Webbook
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	606.52	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.66	J/mol×K	882.32	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method

cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
dvisc	0.0052883	Paxs	606.52	Joback Method
dvisc	0.0049439	Paxs	652.49	Joback Method
dvisc	0.0046630	Paxs	698.45	Joback Method
dvisc	0.0044300	Paxs	744.42	Joback Method
dvisc	0.0042338	Paxs	790.39	Joback Method
dvisc	0.0040664	Paxs	836.35	Joback Method
dvisc	0.0039222	Paxs	882.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C191855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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