

Tetrabenzo[a,f,k,n]perylene

Inchi:	InChI=1S/C36H20/c1-5-13-26-21(9-1)17-25-18-22-10-2-6-14-27(22)35-31-20-24-12-4-8-
InchiKey:	XCUCZRCFIJJYST-UHFFFAOYSA-N
Formula:	C36H20
SMILES:	<chem>c1ccc2c(c1)cc1c3c(cc4cccc4c23)c2c3cccc3cc3cc4cccc4c1c32</chem>
Mol. weight [g/mol]:	452.54
CAS:	128746-59-8

Physical Properties

Property code	Value	Unit	Source
gf	1144.68	kJ/mol	Joback Method
hf	852.97	kJ/mol	Joback Method
hfus	59.44	kJ/mol	Joback Method
hvap	115.12	kJ/mol	Joback Method
log10ws	-15.32		Crippen Method
logp	10.350		Crippen Method
mcvol	342.960	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	1228.76	K	Joback Method
tc	1519.31	K	Joback Method
tf	877.42	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.13	J/molxK	1228.76	Joback Method
cpg	1214.90	J/molxK	1277.19	Joback Method
cpg	1258.52	J/molxK	1325.61	Joback Method
cpg	1307.64	J/molxK	1374.04	Joback Method
cpg	1362.92	J/molxK	1422.46	Joback Method
cpg	1425.02	J/molxK	1470.89	Joback Method
cpg	1494.62	J/molxK	1519.31	Joback Method
dvisc	0.0228438	Paxs	877.42	Joback Method
dvisc	0.0217885	Paxs	935.98	Joback Method

dvisc	0.0208980	Paxs	994.53	Joback Method
dvisc	0.0201371	Paxs	1053.09	Joback Method
dvisc	0.0194799	Paxs	1111.65	Joback Method
dvisc	0.0189069	Paxs	1170.20	Joback Method
dvisc	0.0184030	Paxs	1228.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128746598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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