

Perylo[3,2,1,12-pqrab]perylene

Inchi:	InChI=1S/C34H16/c1-5-17-13-15-25-24-12-4-10-22-20-8-2-6-18-14-16-26-23-11-3-9-21-
InchiKey:	PLUKJIDMXDDKDC-UHFFFAOYSA-N
Formula:	C34H16
SMILES:	<chem>c1cc2ccc3c4ccccc5c6cccc7ccc8c9cccc%10c(c1)c2c3c(c%109)c(c54)c8c76</chem>
Mol. weight [g/mol]:	424.49
CAS:	187-95-1

Physical Properties

Property code	Value	Unit	Source
gf	1207.58	kJ/mol	Joback Method
hf	937.47	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Joback Method
log10ws	-15.37		Crippen Method
logp	9.817		Crippen Method
mcvol	308.220	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	1183.86	K	Joback Method
tc	1465.19	K	Joback Method
tf	918.94	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.98	J/molxK	1183.86	Joback Method
cpg	1086.84	J/molxK	1230.75	Joback Method
cpg	1134.65	J/molxK	1277.64	Joback Method
cpg	1189.14	J/molxK	1324.53	Joback Method
cpg	1251.03	J/molxK	1371.42	Joback Method
cpg	1321.06	J/molxK	1418.30	Joback Method
cpg	1399.93	J/molxK	1465.19	Joback Method
dvisc	0.4024121	Paxs	918.94	Joback Method
dvisc	0.4201945	Paxs	963.09	Joback Method

dvisc	0.4371025	Paxs	1007.25	Joback Method
dvisc	0.4531868	Paxs	1051.40	Joback Method
dvisc	0.4684964	Paxs	1095.55	Joback Method
dvisc	0.4830780	Paxs	1139.71	Joback Method
dvisc	0.4969759	Paxs	1183.86	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=C187951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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