

Benzo[l]cyclopenta[cd]pyrene

Inchi:	InChI=1S/C22H12/c1-2-6-17-16(5-1)18-7-3-4-14-12-15-9-8-13-10-11-19(17)22(20(13)15)
InchiKey:	MEWBBKSDPHWBAG-UHFFFAOYSA-N
Formula:	C22H12
SMILES:	C1=Cc2cc3cccc4c5cccc5c5ccc1c2c5c34
Mol. weight [g/mol]:	276.33
CAS:	113779-16-1

Physical Properties

Property code	Value	Unit	Source
gf	729.98	kJ/mol	Joback Method
hf	557.67	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	6.221		Crippen Method
mcvol	208.380	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	828.86	K	Joback Method
tc	1092.51	K	Joback Method
tf	590.26	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/molxK	828.86	Joback Method
cpg	586.21	J/molxK	872.80	Joback Method
cpg	599.31	J/molxK	916.74	Joback Method
cpg	612.69	J/molxK	960.68	Joback Method
cpg	626.73	J/molxK	1004.62	Joback Method
cpg	641.76	J/molxK	1048.57	Joback Method
cpg	658.14	J/molxK	1092.51	Joback Method
dvisc	0.0083814	Paxs	590.26	Joback Method
dvisc	0.0083273	Paxs	630.03	Joback Method

dvisc	0.0082799	Paxs	669.79	Joback Method
dvisc	0.0082380	Paxs	709.56	Joback Method
dvisc	0.0082008	Paxs	749.33	Joback Method
dvisc	0.0081674	Paxs	789.09	Joback Method
dvisc	0.0081374	Paxs	828.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113779161&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/72-463-8/Benzo-l-cyclopenta-cd-pyrene.pdf>

Generated by Cheméo on 2022-09-24 22:55:32.428510741 +0000 UTC m=+100070.608307798.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.