Cyclopenta(cd)perylene

Inchi: InChI=1S/C22H12/c1-3-13-4-2-6-17-19-12-10-15-8-7-14-9-11-18(22(19)20(14)15)16(5-1)
InchiKey: IVZZWHVVAJTPOG-UHFFFAOYSA-N
Formula: C22H12
SMILES: C1=Cc2ccc3c4cccc5cccc(c6ccc1c2c63)c54
Mol. weight [g/mol]: 276.33
CAS: 189-01-5

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
rinpol	484.70		NIST Webbook
rinpol	3232.00		NIST Webbook
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/mol×K	828.86	Joback Method
cpg	641.76	J/mol×K	1048.57	Joback Method
cpg	626.73	J/mol×K	1004.62	Joback Method
cpg	612.69	J/mol×K	960.68	Joback Method
cpg	599.31	J/mol×K	916.74	Joback Method
cpg	586.21	J/mol×K	872.80	Joback Method
cpg	658.14	J/mol×K	1092.51	Joback Method

dvisc	0.0081374	Pa×s	828.86	Joback Method
dvisc	0.0081674	Pa×s	789.09	Joback Method
dvisc	0.0082008	Pa×s	749.33	Joback Method
dvisc	0.0082380	Pa×s	709.56	Joback Method
dvisc	0.0082799	Pa×s	669.79	Joback Method
dvisc	0.0083273	Pa×s	630.03	Joback Method
dvisc	0.0083814	Pa×s	590.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C189015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume