

1,6-Ethenocyclopenta[cd]pentaleno[2,1,6-gha]per

Inchi:	InChI=1S/C16H16/c1-2-8-10-5-6-12-11-4-3-9-7(1)13(8)16(14(9)11)15(10)12/h1-16H
InchiKey:	BDGDZXGHWJTCIG-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	<chem>C1=CC2C3C=CC4C5C=CC6C1C2C(C65)C34</chem>
Mol. weight [g/mol]:	208.30
CAS:	66081-13-8

Physical Properties

Property code	Value	Unit	Source
gf	531.58	kJ/mol	Joback Method
hf	167.53	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
ie	8.74	eV	NIST Webbook
log10ws	-3.03		Crippen Method
logp	2.899		Crippen Method
mcvol	158.240	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
tb	576.18	K	Joback Method
tc	800.36	K	Joback Method
tf	370.08	K	Joback Method
vc	0.643	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.35	J/molxK	576.18	Joback Method
cpg	494.79	J/molxK	613.54	Joback Method
cpg	514.43	J/molxK	650.91	Joback Method
cpg	532.49	J/molxK	688.27	Joback Method
cpg	549.19	J/molxK	725.64	Joback Method
cpg	564.78	J/molxK	763.00	Joback Method
cpg	579.47	J/molxK	800.36	Joback Method
dvisc	0.0036068	Paxs	370.08	Joback Method

dvisc	0.0071520	Paxs	404.43	Joback Method
dvisc	0.0127403	Paxs	438.78	Joback Method
dvisc	0.0208700	Paxs	473.13	Joback Method
dvisc	0.0319779	Paxs	507.48	Joback Method
dvisc	0.0464172	Paxs	541.83	Joback Method
dvisc	0.0644484	Paxs	576.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66081138&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
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
ie:	Ionization energy
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

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