2,7,8b,3,4b,6-Ethanediylidene dipentaleno[1,6-ab:1',6'-ef]pentalene, hexadecahydro-

Inchi: InChI=1S/C20H20/c1-5-13-7-2-8-14(13)6(1)18-10-3-9-15-11-4-12(16(10)15)20(8,18)19(7
InchiKey: HRQVTWFSLAASTF-UHFFFAOYSA-N
Formula: C20H20
SMILES: C1C2C3C4C1C15C6CC7C8C6C6CC8C8(C3CC4C618)C275
Mol. weight [g/mol]: 260.37
CAS: 89683-62-5

Physical Properties

Property code	Value	Unit	Source
gf	882.56	kJ/mol	Joback Method
hf	384.01	kJ/mol	Joback Method
hfus	34.50	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
ie	8.17	eV	NIST Webbook
log10ws	-3.17		Crippen Method
logp	3.036		Crippen Method
mcvol	173.200	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	653.24	K	Joback Method
tc	884.19	K	Joback Method
tf	632.66	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.28	J/mol×K	845.70	Joback Method
cpg	647.00	J/mol×K	653.24	Joback Method
cpg	665.26	J/mol×K	691.73	Joback Method
cpg	682.88	J/mol×K	730.22	Joback Method
cpg	700.79	J/mol×K	768.72	Joback Method
cpg	719.94	J/mol×K	807.21	Joback Method
cpg	765.75	J/mol×K	884.19	Joback Method
hsubt	90.20 ± 2.30	kJ/mol	445.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89683625&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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