Dicyclopenta[cd,gh]pentalene, 2a,3,3a,5a,6,6a,6b,6c-octahydro-

Inchi: InChI=1S/C12H14/c1-2-8-6-10-4-3-9-5-7(1)11(8)12(9)10/h1-4,7-12H,5-6H2
InchiKey: FGZALOGDPFYZQX-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1=CC2CC3C=CC4CC1C2C43
Mol. weight [g/mol]: 158.24
CAS: 60606-96-4

Physical Properties

Property code	Value	Unit	Source
gf	337.66	kJ/mol	Joback Method
hf	75.07	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
ie	8.25	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.631		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	489.90	K	Joback Method
tc	710.29	K	Joback Method
tf	289.80	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.54	J/mol×K	489.90	Joback Method
cpg	341.07	J/mol×K	526.63	Joback Method
cpg	359.95	J/mol×K	563.36	Joback Method
cpg	377.31	J/mol×K	600.10	Joback Method
cpg	393.29	J/mol×K	636.83	Joback Method
cpg	408.06	J/mol×K	673.56	Joback Method
cpg	421.73	J/mol×K	710.29	Joback Method
dvisc	0.0005230	Pa×s	289.80	Joback Method

dvisc	0.0008339	Pa×s	323.15	Joback Method
dvisc	0.0012184	Pa×s	356.50	Joback Method
dvisc	0.0016684	Pa×s	389.85	Joback Method
dvisc	0.0021742	Pa×s	423.20	Joback Method
dvisc	0.0027258	Pa×s	456.55	Joback Method
dvisc	0.0033138	Pa×s	489.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60606964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
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