

1,2,4-Methenocyclopenta[cd]pentalene-5-carboxaldehyde

Other names: Endrin aldehyde
2,2a,3,3,4,7-hexachlorodecahydro-

InChI: InChI=1S/C12H8Cl6O/c13-8-5-3(2-19)1-4-6(5)9(14,12)(8,17)18)11(16)7(4)10(8,11)15/h2-
(1«alpha»,2«beta»,2a«beta»,4«beta»,4a«beta»,5«beta»)

Formula: C12H8Cl6O

SMILES: O=CC1CC2C3C1C1(Cl)C(Cl)(Cl)C3(Cl)C3(Cl)C2C13Cl

Mol. weight [g/mol]: 380.91

CAS: 7421-93-4

Physical Properties

Property code	Value	Unit	Source
gf	165.21	kJ/mol	Joback Method
hf	-107.89	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.809		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	741.67	K	Joback Method
tc	1011.91	K	Joback Method
tf	648.60	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.57	J/molxK	741.67	Joback Method
cpg	521.79	J/molxK	786.71	Joback Method
cpg	537.66	J/molxK	831.75	Joback Method
cpg	557.37	J/molxK	876.79	Joback Method
cpg	582.08	J/molxK	921.83	Joback Method
cpg	612.98	J/molxK	966.87	Joback Method
cpg	651.24	J/molxK	1011.91	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=C7421934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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.chemeo.com/cid/14-195-0/1-2-4-Methenocyclopenta-cd-pentalene-5-carboxaldehyde-2-2a-3-3-4-7-hexa>

Generated by Cheméo on 2024-04-30 07:41:01.793751951 +0000 UTC m=+16752110.714329266.

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