

1,2,4-Ethanylylidene-1H-cyclobuta[cd]pentalene, c

Other names:	1,2,4-Ethanylylidene-1H-cyclobuta[cd]pentalene, octahydro-5-methyl-7-methylene, (1 «alph
Inchi:	InChI=1S/C13H16/c1-4-8-6-3-7-9(8)5(2)11-10(4)12(6)13(7)11/h5-13H,1,3H2,2H3
InchiKey:	REFUZKMRSXPUBN-UHFFFAOYSA-N
Formula:	C13H16
SMILES:	C=C1C2C3CC4C2C(C)C2C1C3C42
Mol. weight [g/mol]:	172.27
CAS:	42607-64-7

Physical Properties

Property code	Value	Unit	Source
gf	432.97	kJ/mol	Joback Method
hf	79.87	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	42.33	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.566		Crippen Method
mcvol	135.430	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
tb	493.94	K	Joback Method
tc	693.27	K	Joback Method
tf	336.77	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.96	J/molxK	493.94	Joback Method
cpg	389.90	J/molxK	527.16	Joback Method
cpg	408.35	J/molxK	560.38	Joback Method
cpg	425.44	J/molxK	593.61	Joback Method
cpg	441.30	J/molxK	626.83	Joback Method
cpg	456.07	J/molxK	660.05	Joback Method
cpg	469.88	J/molxK	693.27	Joback Method
dvisc	0.0009407	Paxs	336.77	Joback Method

dvisc	0.0018052	Paxs	362.96	Joback Method
dvisc	0.0031730	Paxs	389.16	Joback Method
dvisc	0.0051943	Paxs	415.36	Joback Method
dvisc	0.0080201	Paxs	441.55	Joback Method
dvisc	0.0117952	Paxs	467.75	Joback Method
dvisc	0.0166518	Paxs	493.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C42607647&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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