

4,2,7-Ethanylylidencyclopenta[b]pyran-9-one,

Other names: 9-Oxatetracyclo[5.4.0.0(3.10).0(4,8)]undeca-5-en-2-one

InChI: InChI=1S/C10H10O2/c11-9-6-3-7-8(9)5-2-1-4(6)10(5)12-7/h1-2,4-8,10H,3H2

InchiKey: NXSDNHMBWHSSKO-UHFFFAOYSA-N

Formula: C10H10O2

SMILES: O=C1C2CC3OC4C2C=CC4C13

Mol. weight [g/mol]: 162.19

CAS: 65181-92-2

Physical Properties

Property code	Value	Unit	Source
chs	-5121.70 ± 1.20	kJ/mol	NIST Webbook
gf	94.25	kJ/mol	Joback Method
hf	-204.97	kJ/mol	Joback Method
hfs	-242.50 ± 1.50	kJ/mol	NIST Webbook
hfus	27.15	kJ/mol	Joback Method
hsub	96.00 ± 1.50	kJ/mol	NIST Webbook
hvap	45.77	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.775		Crippen Method
mcvol	111.460	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	535.48	K	Joback Method
tc	767.18	K	Joback Method
tf	364.81	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.13	J/molxK	535.48	Joback Method
cpg	327.02	J/molxK	574.10	Joback Method
cpg	342.59	J/molxK	612.71	Joback Method
cpg	356.95	J/molxK	651.33	Joback Method
cpg	370.24	J/molxK	689.94	Joback Method

cpg	382.58	J/mol×K	728.56	Joback Method
cpg	394.10	J/mol×K	767.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65181922&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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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