Octahydro-1,2,4-metheno-3H-cyclobuta [cd] pentalen-3-one

Inchi: InChI=1S/C10H10O/c11-10-7-3-1-2-4-5(3)9(10)8(4)6(2)7/h2-9H,1H2
InchiKey: KIOXQCAVQTVNCR-UHFFFAOYSA-N
Formula: C10H10O
SMILES: O=C1C2C3CC4C2C2C1C3C42
Mol. weight [g/mol]: 146.19
CAS: 15443-37-5

Physical Properties

Property code	Value	Unit	Source
chs	-5417.02	kJ/mol	NIST Webbook
gf	251.85	kJ/mol	Joback Method
hf	-53.65	kJ/mol	Joback Method
hfs	52.72	kJ/mol	NIST Webbook
hfus	25.55	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.943		Crippen Method
mcvol	99.030	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	494.36	K	Joback Method
tc	709.53	K	Joback Method
tf	365.26	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.72	J/mol×K	494.36	Joback Method
cpg	299.51	J/mol×K	530.22	Joback Method
cpg	314.86	J/mol×K	566.08	Joback Method
cpg	328.93	J/mol×K	601.94	Joback Method
cpg	341.87	J/mol×K	637.81	Joback Method
cpg	353.84	J/mol×K	673.67	Joback Method
cpg	364.99	J/mol×K	709.53	Joback Method

Sources

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=C15443375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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