5-Oxo-«delta»4-decahydrobenzindene

Inchi: InChI=1S/C13H18O/c14-12-7-3-5-10-8-9-4-1-2-6-11(9)13(10)12/h3,7,9-11,13H,1-2,4-6,8
InchiKey: VGIGCWNCMHCEMC-UHFFFAOYSA-N
Formula: C13H18O
SMILES: O=C1C=CCC2CC3CCCCC3C12
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	92.09	kJ/mol	Joback Method
hf	-218.15	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.958		Crippen Method
mcvol	158.720	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	596.45	K	Joback Method
tc	841.69	K	Joback Method
tf	340.75	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.56	J/mol×K	596.45	Joback Method
cpg	467.82	J/mol×K	637.32	Joback Method
cpg	489.44	J/mol×K	678.20	Joback Method
cpg	509.49	J/mol×K	719.07	Joback Method
cpg	528.05	J/mol×K	759.95	Joback Method
cpg	545.18	J/mol×K	800.82	Joback Method
cpg	560.97	J/mol×K	841.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U8187&Units=SI

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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