

Spiro[4.5]dec-6-ene-8-one

Inchi:

InChI=1S/C10H14O/c11-9-3-7-10(8-4-9)5-1-2-6-10/h3,7H,1-2,4-6,8H2

InchiKey:

XKYBFVHJBMGXPO-UHFFFAOYSA-N

Formula:

C10H14O

SMILES:

O=C1C=CC2(CCCC2)CC1

Mol. weight [g/mol]:

150.22

CAS:

14523-53-6

Physical Properties

Property code	Value	Unit	Source
gf	16.01	kJ/mol	Joback Method
hf	-173.11	kJ/mol	Joback Method
hfus	2.89	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.466		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	530.65	K	Joback Method
tc	783.47	K	Joback Method
tf	321.38	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.83	J/mol×K	530.65	Joback Method
cpg	325.21	J/mol×K	572.79	Joback Method
cpg	343.13	J/mol×K	614.92	Joback Method
cpg	359.76	J/mol×K	657.06	Joback Method
cpg	375.30	J/mol×K	699.20	Joback Method
cpg	389.92	J/mol×K	741.34	Joback Method
cpg	403.80	J/mol×K	783.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C14523536&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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