

Spiro[5.5]undeca-1,8-dien-3-one

Inchi:	InChI=1S/C11H14O/c12-10-4-8-11(9-5-10)6-2-1-3-7-11/h1-2,4,8H,3,5-7,9H2
InchiKey:	WFZMDPXIOJHKJV-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	O=C1C=CC2(CC=CCC2)CC1
Mol. weight [g/mol]:	162.23
CAS:	30834-47-0

Physical Properties

Property code	Value	Unit	Source
gf	42.29	kJ/mol	Joback Method
hf	-142.13	kJ/mol	Joback Method
hfus	4.60	kJ/mol	Joback Method
hvap	44.75	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.632		Crippen Method
mcvol	137.100	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	556.96	K	Joback Method
tc	816.60	K	Joback Method
tf	329.89	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.32	J/mol×K	556.96	Joback Method
cpg	355.15	J/mol×K	600.23	Joback Method
cpg	373.49	J/mol×K	643.51	Joback Method
cpg	390.52	J/mol×K	686.78	Joback Method
cpg	406.44	J/mol×K	730.06	Joback Method
cpg	421.44	J/mol×K	773.33	Joback Method
cpg	435.71	J/mol×K	816.60	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=C30834470&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
mccol:	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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