

Spiro-2-cyclohexene-4-one-1,2'-(5-norbornene)

Inchi:	InChI=1S/C12H14O/c13-11-3-5-12(6-4-11)8-9-1-2-10(12)7-9/h1-3,5,9-10H,4,6-8H2
InchiKey:	ZANBBQSNIRIMCX-UHFFFAOYSA-N
Formula:	C12H14O
SMILES:	O=C1C=CC2(CC1)CC1C=CC2C1
Mol. weight [g/mol]:	174.24
CAS:	30834-51-6

Physical Properties

Property code	Value	Unit	Source
gf	127.95	kJ/mol	Joback Method
hf	-97.99	kJ/mol	Joback Method
hfus	10.60	kJ/mol	Joback Method
hvap	46.24	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.488		Crippen Method
mcvol	140.330	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	573.37	K	Joback Method
tc	828.08	K	Joback Method
tf	361.90	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.21	J/molxK	573.37	Joback Method
cpg	388.91	J/molxK	615.82	Joback Method
cpg	407.06	J/molxK	658.27	Joback Method
cpg	423.92	J/molxK	700.72	Joback Method
cpg	439.72	J/molxK	743.18	Joback Method
cpg	454.72	J/molxK	785.63	Joback Method
cpg	469.14	J/molxK	828.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30834516&Units=SI
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

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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