

spiro[adamantane-2,1'-cyclopropane]

Inchi: InChI=1S/C12H18/c1-2-12(1)10-4-8-3-9(6-10)7-11(12)5-8/h8-11H,1-7H2
InchiKey: ZYIPFTBWBGOVBV-UHFFFAOYSA-N
Formula: C12H18
SMILES: C1C2CC3CC1CC(C2)C31CC1
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	279.96	kJ/mol	Joback Method
hf	-4.91	kJ/mol	Joback Method
hfus	14.15	kJ/mol	Joback Method
hvap	40.50	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.223		Crippen Method
mcvol	136.500	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
ripol	1272.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1477.00		NIST Webbook
tb	496.49	K	Joback Method
tc	722.10	K	Joback Method
tf	316.42	K	Joback Method
vc	0.532	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.23	J/molxK	496.49	Joback Method
cpg	376.85	J/molxK	534.09	Joback Method

cpg	397.46	J/mol×K	571.69	Joback Method
cpg	416.33	J/mol×K	609.29	Joback Method
cpg	433.71	J/mol×K	646.90	Joback Method
cpg	449.85	J/mol×K	684.50	Joback Method
cpg	465.02	J/mol×K	722.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R304888&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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