

(Dispiro[bicyclo[2.2.1]hepta-2,5-diene-7,1'-cyclopropane-2',7''-bicyclo[2.2.1]hepta[2,5]diene])

Inchi:	InChI=1S/C15H14/c1-2-11-4-3-10(1)14(11)9-15(14)12-5-6-13(15)8-7-12/h1-8,10-13H,9H
InchiKey:	YVIYAEURKSYKGY-UHFFFAOYSA-N
Formula:	C15H14
SMILES:	C1=CC2C=CC1C21CC12C1C=CC2C=C1
Mol. weight [g/mol]:	194.27
CAS:	73045-27-9

Physical Properties

Property code	Value	Unit	Source
gf	480.32	kJ/mol	Joback Method
hf	252.33	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	47.11	kJ/mol	Joback Method
ie	8.25	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-3.54		Crippen Method
logp	3.107		Crippen Method
mcvol	150.710	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	568.75	K	Joback Method
tc	818.92	K	Joback Method
tf	395.11	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.52	J/molxK	568.75	Joback Method
cpg	432.53	J/molxK	610.44	Joback Method
cpg	449.57	J/molxK	652.14	Joback Method
cpg	465.18	J/molxK	693.83	Joback Method
cpg	479.91	J/molxK	735.53	Joback Method
cpg	494.31	J/molxK	777.22	Joback Method
cpg	508.91	J/molxK	818.92	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=C73045279&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
h vap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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