

Benzonorbornene, 9-isopropylidene-

Inchi:	InChI=1S/C14H16/c1-9(2)14-12-7-8-13(14)11-6-4-3-5-10(11)12/h3-6,12-13H,7-8H2,1-2H
InchiKey:	LKPODQYMUXPGQW-UHFFFAOYSA-N
Formula:	C14H16
SMILES:	CC(C)=C1C2CCC1c1ccccc12
Mol. weight [g/mol]:	184.28
CAS:	7350-77-8

Physical Properties

Property code	Value	Unit	Source
gf	340.29	kJ/mol	Joback Method
hf	110.77	kJ/mol	Joback Method
hfus	23.05	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-4.32		Crippen Method
logp	3.998		Crippen Method
mcvol	158.340	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
tb	567.11	K	Joback Method
tc	795.61	K	Joback Method
tf	322.28	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.83	J/molxK	567.11	Joback Method
cpg	412.69	J/molxK	605.19	Joback Method
cpg	429.23	J/molxK	643.28	Joback Method
cpg	444.58	J/molxK	681.36	Joback Method
cpg	458.86	J/molxK	719.44	Joback Method
cpg	472.19	J/molxK	757.53	Joback Method
cpg	484.72	J/molxK	795.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7350778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
ie:	Ionization energy
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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