5-Norbornen-2-one

Other names: Bicyclo(2.2.1)hept-5-en-2-one
Dehydronorcamphor
Norcamphor, dehydro-
2-Norbornen-5-one
2-Norbornenone
5-Norbornen-2-one

Inchi: InChI=1S/C7H8O/c8-7-4-5-1-2-6(7)3-5/h1-2,5-6H,3-4H2

InchiKey: HUQXEIFQYCVOPD-UHFFFAOYSA-N

Formula: C7H8O

SMILES: O=C1CC2C=CC1C2

Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
affp	845.30	kJ/mol	NIST Webbook
basg	813.40	kJ/mol	NIST Webbook
hf	-47.63	kJ/mol	Cheméo Relay (1.0)
hfus	8.79	kJ/mol	Joback Method
hvap	46.19	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	NIST Webbook
ie	8.90 ± 0.02	eV	NIST Webbook
logp	1.151		Crippen Method
mcvol	85.040	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	931.00		NIST Webbook
rinpol	931.00		NIST Webbook
tb	431.31	K	Cheméo Relay (1.0)
tc	676.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.45	J/mol×K	444.29	Joback Method
cpg	190.19	J/mol×K	482.08	Joback Method

cpg	203.08	J/mol×K	519.86	Joback Method
cpg	215.13	J/mol×K	557.65	Joback Method
cpg	226.41	J/mol×K	595.44	Joback Method
cpg	236.95	J/mol×K	633.22	Joback Method
cpg	246.79	J/mol×K	671.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C694984&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature