2,4,6-Cycloheptatrien-1-one

Other names:	Tropone
	Cycloheptatrienone
	Tropon
	2,4,6-Cycloheptatriene-1-one
Inchi:	InChI=1S/C7H6O/c8-7-5-3-1-2-4-6-7/h1-6H
InchiKey:	QVWDCTQRORVHHT-UHFFFAOYSA-N
Formula:	C7H6O
SMILES:	O=c1ccccc1
Mol. weight [g/mol]:	106.12
CAS:	539-80-0

Physical Properties

Property code	Value	Unit	Source
affp	920.80	kJ/mol	NIST Webbook
basg	891.00	kJ/mol	NIST Webbook
chl	-3602.00 ± 3.00	kJ/mol	NIST Webbook
ie	8.88 ± 0.05	eV	NIST Webbook
ie	9.68 ± 0.02	eV	NIST Webbook
ie	8.89 ± 0.03	eV	NIST Webbook
ie	8.90 ± 0.02	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-0.89		Crippen Method
logp	1.047		Crippen Method
mcvol	87.300	ml/mol	McGowan Method
rinpol	1182.00		NIST Webbook
tf	268.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	54.20	kJ/mol	298.00	NIST Webbook
hvapt	54.00 ± 0.40	kJ/mol	297.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C539800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point