Oxepane

Other names:	Hexahydrooxepin
	Hexamethylene oxide
	Hexane, 1,6-epoxy-
	Oxacycloheptane
	Oxepin, hexahydro-
Inchi:	InChI=1S/C6H12O/c1-2-4-6-7-5-3-1/h1-6H2
InchiKey:	UHHKSVZZTYJVEG-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C1CCCOCC1
Mol. weight [g/mol]:	100.16
CAS:	592-90-5

Physical Properties

Property code	Value	Unit	Source
affp	834.20	kJ/mol	NIST Webbook
basg	806.80	kJ/mol	NIST Webbook
gf	-66.42	kJ/mol	Joback Method
hf	-230.67	kJ/mol	Joback Method
hfus	7.94	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
ie	9.15 ± 0.05	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.577		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
rinpol	804.00		NIST Webbook
rinpol	804.00		NIST Webbook
tb	389.15 ± 1.00	K	NIST Webbook
tc	606.54	K	Joback Method
tf	192.05	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.77	J/mol×K	392.12	Joback Method
cpg	177.11	J/mol×K	427.86	Joback Method
cpg	191.68	J/mol×K	463.59	Joback Method
cpg	205.49	J/mol×K	499.33	Joback Method
cpg	218.56	J/mol×K	535.07	Joback Method
cpg	230.91	J/mol×K	570.80	Joback Method
cpg	242.55	J/mol×K	606.54	Joback Method
dvisc	0.0287555	Pa×s	192.05	Joback Method
dvisc	0.0078368	Pa×s	225.40	Joback Method
dvisc	0.0029859	Pa×s	258.74	Joback Method
dvisc	0.0014181	Pa×s	292.09	Joback Method
dvisc	0.0007845	Pa×s	325.43	Joback Method
dvisc	0.0004845	Pa×s	358.77	Joback Method
dvisc	0.0003248	Pa×s	392.12	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C592905&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume