1,3-Dioxepin, 4,7-dihydro-

Other names: 4,7-Dihydro-1,3-dioxepin
Inchi: InChI=1S/C5H8O2/c1-2-4-7-5-6-3-1/h1-2H,3-5H2
InchiKey: BAKUAUDFCNFLBX-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: C1=CCOCOC1
Mol. weight [g/mol]: 100.12
CAS: 5417-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-131.00	kJ/mol	Joback Method
hf	-284.25	kJ/mol	Joback Method
hfus	14.55	kJ/mol	Joback Method
hvap	36.95	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
log10ws	-0.33		Crippen Method
logp	0.547		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
tb	399.20	K	NIST Webbook
tc	614.53	K	Joback Method
tf	208.11	K	Joback Method
vc	0.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.96	J/mol×K	395.35	Joback Method
cpg	194.21	J/mol×K	578.00	Joback Method
cpg	184.60	J/mol×K	541.47	Joback Method
cpg	174.38	J/mol×K	504.94	Joback Method
cpg	163.55	J/mol×K	468.41	Joback Method
cpg	152.08	J/mol×K	431.88	Joback Method

cpg	203.22	J/mol×K	614.53	Joback Method
dvisc	0.0003571	Pa×s	395.35	Joback Method
dvisc	0.0005189	Pa×s	364.14	Joback Method
dvisc	0.0008089	Pa×s	332.94	Joback Method
dvisc	0.0013821	Pa×s	301.73	Joback Method
dvisc	0.0026724	Pa×s	270.52	Joback Method
dvisc	0.0061364	Pa×s	239.32	Joback Method
dvisc	0.0180802	Pa×s	208.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5417323&Units=SI
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

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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