

1,3-Dioxepin

Inchi:	InChI=1S/C5H6O2/c1-2-4-7-5-6-3-1/h1-4H,5H2
InchiKey:	GTPWYANJPNGAAY-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	C1=COCOC=C1
Mol. weight [g/mol]:	98.10
CAS:	291-92-9

Physical Properties

Property code	Value	Unit	Source
gf	-101.04	kJ/mol	Joback Method
hf	-226.47	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	37.24	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.18		Crippen Method
logp	1.018		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	5243.40	kPa	Joback Method
tb	394.51	K	Joback Method
tc	616.11	K	Joback Method
tf	208.87	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.60	J/mol×K	394.51	Joback Method
cpg	138.26	J/mol×K	431.44	Joback Method
cpg	148.31	J/mol×K	468.38	Joback Method
cpg	157.76	J/mol×K	505.31	Joback Method
cpg	166.63	J/mol×K	542.24	Joback Method
cpg	174.93	J/mol×K	579.18	Joback Method
cpg	182.68	J/mol×K	616.11	Joback Method

dvisc	0.0131689	Pa×s	208.87	Joback Method
dvisc	0.0048151	Pa×s	239.81	Joback Method
dvisc	0.0022158	Pa×s	270.75	Joback Method
dvisc	0.0011956	Pa×s	301.69	Joback Method
dvisc	0.0007236	Pa×s	332.63	Joback Method
dvisc	0.0004770	Pa×s	363.57	Joback Method
dvisc	0.0003357	Pa×s	394.51	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=C291929&Units=SI

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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