

2H-Pyran

Inchi:	InChI=1S/C5H6O/c1-2-4-6-5-3-1/h1-4H,5H2
InchiKey:	MGADZUXDNSDTHW-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	C1=CCOC=C1
Mol. weight [g/mol]:	82.10

Physical Properties

Property code	Value	Unit	Source
gf	-2.82	kJ/mol	Joback Method
hf	-88.31	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	32.56	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.087		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
ripol	1775.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	363.29	K	Joback Method
tc	574.83	K	Joback Method
tf	185.82	K	Joback Method
vc	0.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.38	J/molxK	363.29	Joback Method
cpg	114.49	J/molxK	398.55	Joback Method
cpg	123.99	J/molxK	433.80	Joback Method
cpg	132.92	J/molxK	469.06	Joback Method
cpg	141.29	J/molxK	504.32	Joback Method
cpg	149.12	J/molxK	539.58	Joback Method
cpg	156.44	J/molxK	574.83	Joback Method
dvisc	0.0070354	Paxs	185.82	Joback Method

dvisc	0.0029231	Paxs	215.40	Joback Method
dvisc	0.0015014	Paxs	244.98	Joback Method
dvisc	0.0008902	Paxs	274.55	Joback Method
dvisc	0.0005843	Paxs	304.13	Joback Method
dvisc	0.0004133	Paxs	333.71	Joback Method
dvisc	0.0003092	Paxs	363.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R557290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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