

1,3-Dioxolane, 2-propyl-

Other names:	Butanal, cyclic 1,2-ethanediyl acetal 2-Propyl-1,3-dioxolane 2-Propyldioxolane
Inchi:	InChI=1S/C6H12O2/c1-2-3-6-7-4-5-8-6/h6H,2-5H2,1H3
InchiKey:	JSDUOUVZQRZOOY-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCC1OCCO1
Mol. weight [g/mol]:	116.16
CAS:	3390-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-136.05	kJ/mol	Joback Method
hf	-370.69	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	38.23	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.159		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	870.00		NIST Webbook
rinpol	832.00		NIST Webbook
tb	405.86	K	Joback Method
tc	602.78	K	Joback Method
tf	221.42	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.75	J/mol×K	405.86	Joback Method
cpg	254.87	J/mol×K	569.96	Joback Method
cpg	244.04	J/mol×K	537.14	Joback Method
cpg	232.63	J/mol×K	504.32	Joback Method

cpg	220.63	J/mol×K	471.50	Joback Method
cpg	208.01	J/mol×K	438.68	Joback Method
cpg	265.14	J/mol×K	602.78	Joback Method
dvisc	0.0004266	Pa×s	405.86	Joback Method
dvisc	0.0005480	Pa×s	375.12	Joback Method
dvisc	0.0007360	Pa×s	344.38	Joback Method
dvisc	0.0010475	Pa×s	313.64	Joback Method
dvisc	0.0016097	Pa×s	282.90	Joback Method
dvisc	0.0027467	Pa×s	252.16	Joback Method
dvisc	0.0054364	Pa×s	221.42	Joback Method

Sources

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=C3390134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

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