

1,3-Dioxolane, 4-methyl-2-(1-methylethyl), cis

Other names:	1,3-Dioxolane, 4-methyl-2-(1-methylethyl), trans 2-isopropyl-4-methyl-1,3-dioxolane
Inchi:	InChI=1S/C7H14O2/c1-5(2)7-8-4-6(3)9-7/h5-7H,4H2,1-3H3
InchiKey:	NWXXKKDLGZLEGH-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CC1COC(C(C)C)O1
Mol. weight [g/mol]:	130.18
CAS:	67879-60-1

Physical Properties

Property code	Value	Unit	Source
gf	-137.78	kJ/mol	Joback Method
hf	-416.95	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	39.76	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.404		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	835.00		NIST Webbook
tb	423.63	K	Joback Method
tc	622.94	K	Joback Method
tf	213.45	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.22	J/mol×K	423.63	Joback Method
cpg	304.15	J/mol×K	589.72	Joback Method
cpg	291.70	J/mol×K	556.50	Joback Method
cpg	278.59	J/mol×K	523.28	Joback Method
cpg	264.82	J/mol×K	490.07	Joback Method
cpg	250.36	J/mol×K	456.85	Joback Method
cpg	315.97	J/mol×K	622.94	Joback Method
dvisc	0.0003894	Pa×s	423.63	Joback Method
dvisc	0.0004946	Pa×s	388.60	Joback Method
dvisc	0.0006588	Pa×s	353.57	Joback Method
dvisc	0.0009346	Pa×s	318.54	Joback Method
dvisc	0.0014455	Pa×s	283.51	Joback Method
dvisc	0.0025283	Pa×s	248.48	Joback Method
dvisc	0.0053129	Pa×s	213.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67879601&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
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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