

1,3-Dioxolane, 2-(1-methylpropyl)-

Other names:	1,3-Dioxolane, 2-sec-butyl-
Inchi:	InChI=1S/C7H14O2/c1-3-6(2)7-8-4-5-9-7/h6-7H,3-5H2,1-2H3
InchiKey:	FRBNVSJPLIGZIP-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(C)C1OCCO1
Mol. weight [g/mol]:	130.18
CAS:	14447-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-130.07	kJ/mol	Joback Method
hf	-396.61	kJ/mol	Joback Method
hfus	20.26	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.405		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	901.00		NIST Webbook
tb	428.30	K	Joback Method
tc	628.03	K	Joback Method
tf	217.69	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.85	J/molxK	428.30	Joback Method
cpg	302.13	J/molxK	594.74	Joback Method
cpg	290.05	J/molxK	561.46	Joback Method
cpg	277.31	J/molxK	528.17	Joback Method
cpg	263.87	J/molxK	494.88	Joback Method

cpg	249.72	J/molxK	461.59	Joback Method
cpg	313.56	J/molxK	628.03	Joback Method
dvisc	0.0003974	Paxs	428.30	Joback Method
dvisc	0.0005289	Paxs	393.20	Joback Method
dvisc	0.0007446	Paxs	358.10	Joback Method
dvisc	0.0011292	Paxs	323.00	Joback Method
dvisc	0.0018954	Paxs	287.89	Joback Method
dvisc	0.0036737	Paxs	252.79	Joback Method
dvisc	0.0088142	Paxs	217.69	Joback Method

Sources

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=C14447257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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