

1,3-Dioxolane, 4-methyl-2-(1-methylpropyl), trans

Inchi:	InChI=1S/C8H16O2/c1-4-6(2)8-9-5-7(3)10-8/h6-8H,4-5H2,1-3H3/t6?,7-,8-/m0/s1
InchiKey:	MQZVWFKZBQTGMS-ALKRTJFJSA-N
Formula:	C8H16O2
SMILES:	CCC(C)C1OCC(C)O1
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
gf	-129.36	kJ/mol	Joback Method
hf	-437.59	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.794		Crippen Method
mcvol	124.460	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	933.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	938.00		NIST Webbook
tb	446.51	K	Joback Method
tc	643.69	K	Joback Method
tf	224.72	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.45	J/mol×K	446.51	Joback Method
cpg	351.27	J/mol×K	610.82	Joback Method
cpg	337.94	J/mol×K	577.96	Joback Method
cpg	323.91	J/mol×K	545.10	Joback Method
cpg	309.16	J/mol×K	512.24	Joback Method
cpg	293.68	J/mol×K	479.37	Joback Method
cpg	363.92	J/mol×K	643.69	Joback Method

dvisc	0.0003810	Pa×s	446.51	Joback Method
dvisc	0.0004874	Pa×s	409.54	Joback Method
dvisc	0.0006547	Pa×s	372.58	Joback Method
dvisc	0.0009386	Pa×s	335.62	Joback Method
dvisc	0.0014712	Pa×s	298.65	Joback Method
dvisc	0.0026179	Pa×s	261.69	Joback Method
dvisc	0.0056311	Pa×s	224.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R69877&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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