

1,3-Dioxolane, 4-ethyl-2-methyl, trans

Inchi:	InChI=1S/C6H12O2/c1-3-6-4-7-5(2)8-6/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey:	PXOMUGHKQXQZIV-WDSKDSINSA-N
Formula:	C6H12O2
SMILES:	CCC1COC(C)O1
Mol. weight [g/mol]:	116.16

Physical Properties

Property code	Value	Unit	Source
gf	-143.76	kJ/mol	Joback Method
hf	-391.03	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	37.92	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpola	762.00		NIST Webbook
rinpola	762.00		NIST Webbook
rinpola	774.00		NIST Webbook
rinpola	770.00		NIST Webbook
tb	401.19	K	Joback Method
tc	597.60	K	Joback Method
tf	217.18	K	Joback Method
vc	0.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.22	J/molxK	401.19	Joback Method
cpg	208.70	J/molxK	433.92	Joback Method
cpg	221.59	J/molxK	466.66	Joback Method
cpg	233.89	J/molxK	499.39	Joback Method
cpg	245.63	J/molxK	532.13	Joback Method
cpg	256.80	J/molxK	564.86	Joback Method

cpg	267.43	J/molxK	597.60	Joback Method
dvisc	0.0032903	Paxs	217.18	Joback Method
dvisc	0.0018693	Paxs	247.85	Joback Method
dvisc	0.0012029	Paxs	278.52	Joback Method
dvisc	0.0008448	Paxs	309.19	Joback Method
dvisc	0.0006323	Paxs	339.85	Joback Method
dvisc	0.0004966	Paxs	370.52	Joback Method
dvisc	0.0004046	Paxs	401.19	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=R69859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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