

cis-2-Thyl-4-methyl-1,3-dioxolane

Other names:	1,3-Dioxolane, 2-ethyl-4-methyl-, (2R,4S)-rel- 1,3-Dioxolane, 2-ethyl-4-methyl-, cis-
Inchi:	InChI=1S/C6H12O2/c1-3-6-7-4-5(2)8-6/h5-6H,3-4H2,1-2H3
InchiKey:	CSZCLQLJVFLXLI-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC1OCC(C)O1
Mol. weight [g/mol]:	116.16
CAS:	1568-99-6

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
tb	401.19	K	Joback Method
tc	597.60	K	Joback Method
tf	217.18	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.22	J/mol×K	401.19	Joback Method
cpg	256.80	J/mol×K	564.86	Joback Method
cpg	245.63	J/mol×K	532.13	Joback Method
cpg	233.89	J/mol×K	499.39	Joback Method
cpg	221.59	J/mol×K	466.66	Joback Method
cpg	208.70	J/mol×K	433.92	Joback Method
cpg	267.43	J/mol×K	597.60	Joback Method

dvisc	0.0004046	Pa×s	401.19	Joback Method
dvisc	0.0004966	Pa×s	370.52	Joback Method
dvisc	0.0006323	Pa×s	339.85	Joback Method
dvisc	0.0008448	Pa×s	309.19	Joback Method
dvisc	0.0012029	Pa×s	278.52	Joback Method
dvisc	0.0018693	Pa×s	247.85	Joback Method
dvisc	0.0032903	Pa×s	217.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1568996&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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